| HEADER | | | | | | | | | | MTGL |
|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1 | CB | ALA | 1 | 15.214 | -2.789 | 18.265 | 1.00 | 29.91 | MTGL |
| ATOM | 2 | C | ALA | 1 | 17.670 | -3.053 | 17.823 | 1.00 | 27.24 | MTGL |
| ATOM | 3 | O | ALA | 1 | 18.335 | -2.394 | 17.026 | 1.00 | 27.44 | MTGL |
| ATOM | 4 | N | ALA | 1 | 16.132 | -5.006 | 17.678 | 1.00 | 29.26 | MTGL |
| ATOM | 5 | CA | ALA | 1 | 16.268 | -3.540 | 17.450 | 1.00 | 28.32 | MTGL |
| ATOM | 6 | N | LEU | 2 | 18.116 | -3.378 | 19.034 | 1.00 | 25.13 | MTGL |
| ATOM | 7 | CA | LEU | 2 | 19.439 | -2.955 | 19.486 | 1.00 | 23.17 | MTGL |
| ATOM | 8 | CB | LEU | 2 | 19.648 | -3.322 | 20.957 | 1.00 | 23.07 | MTGL |
| ATOM | 9 | CG | LEU | 2 | 18.891 | -2.507 | 22.005 | 1.00 | 23.57 | MTGL |
| ATOM | 10 | CD1 | LEU | 2 | 19.156 | -3.090 | 23.384 | 1.00 | 23.95 | MTGL |
| ATOM | 11 | CD2 | LEU | 2 | 19.330 | -1.057 | 21.940 | 1.00 | 23.31 | MTGL |
| ATOM | 12 | C | LEU | 2 | 20.560 | -3.574 | 18.664 | 1.00 | 22.07 | MTGL |
| ATOM | 13 | O | LEU | 2 | 20.524 | -4.757 | 18.340 | 1.00 | 21.83' | MTGL |
| ATOM | 14 | N | THR | 3 | 21.557 | -2.767 | 18.329 | 1.00 | 20.29 | MTGL |
| ATOM | 15 | CA | THR | 3 | 22.699 | -3.257 | 17.575 | 1.00 | 19.63 | MTGL |
| ATOM | 16 | CB | THR | 3 | 23.506 | -2.100 | 16.978 | 1.00 | 20.33 | MTGL |
| ATOM | 17 | OG1 | THR | 3 | 22.674 | -1.360 | 16.083 | 1.00 | 20.92 | MTGL |
| ATOM | 18 | CG2 | THR | 3 | 24.728 | -2.626 | 16.227 | 1.00 | 20.96 | MTGL |
| ATOM | 19 | C | THR | 3 | 23.610 | -4.038 | 18.515 | 1.00 | 19.16 | MTGL |
| ATOM | 20 | O | THR | 3 | 24.131 | -5.092 | 18.156 | 1.00 | 19.29 | MTGL |
| ATOM | 21 | N | TYR | 4 | 23.796 | -3.514 | 19.724 | 1.00 | 18.09 | MTGL |
| ATOM | 22 | CA | TYR | 4 | 24.652 | -4.159 | 20.715 | 1.00 | 17.42 | MTGL |
| ATOM | 23 | CB | TYR | 4 | 25.724 | -3.180 | 21.202 | 1.00 | 17.15 | MTGL |
| ATOM | 24 | CG | TYR | 4 | 26.514 | -2.544 | 20.082 | 1.00 | 18.02 | MTGL |
| ATOM | 25 | CD1 | TYR | 4 | 27.516 | -3.251 | 19.412 | 1.00 | 17.43 | MTGL |
| ATOM | 26 | CE1 | TYR | 4 | 28.210 | -2.678 | 18.348 | 1.00 | 18.07 | MTGL |
| ATOM | 27 | CD2 | TYR | 4 | 26.229 | -1.246 | 19.661 | 1.00 | 17.07 | MTGL |
| ATOM | 28 | CE2 | TYR | 4 | 26.916 | -0.666 | 18.598 | 1.00 | 18.55 | MTGL |
| ATOM | 29 | CZ | TYR | 4 | 27.902 | -1.386 | 17.948 | 1.00 | 17.59 | MTGL |
| ATOM | 30 | OH | TYR | 4 | 28.564 | -0.814 | 16.891 | 1.00 | 18.07 | MTGL |
| ATOM | 31 | C | TYR | 4 | 23.858 | -4.657 | 21.912 | 1.00 | 16.29 | MTGL |
| ATOM | 32 | O | TYR | 4 | 23.210 | -3.876 | 22.615 | 1.00 | 16.95 | MTGL |
| ATOM | 33 | N | ARG | 5 | 23.907 | -5.964 | 22.125 | 1.00 | 15.87 | MTGL |
| ATOM | 34 | CA | ARG | 5 | 23.232 | -6.611 | 23.244 | 1.00 | 16.37 | MTGL |
| ATOM | 35 | CB | ARG | 5 | 22.281 | -7.711 | 22.746 | 1.00 | 17.04 | MTGL |
| ATOM | 36 | CG | ARG | 5 | 21.203 | -7.235 | 21.764 | 1.00 | 18.21 | MTGL |
| ATOM | 37 | CD | ARG | 5 | 20.189 | -8.348 | 21.482 | 1.00 | 18.30 | MTGL |
| ATOM | 38 | NE | ARG | 5 | 20.839 | -9.547 | 20.950 | 1.00 | 19.36 | MTGL |
| ATOM | 39 | CZ | ARG | 5 | 21.243 | -9.681 | 19.692 | 1.00 | 20.62 | MTGL |
| ATOM | 40 | NH1 | ARG | 5 | 21.054 | -8.696 | 18.824 | 1.00 | 19.45 | MTGL |
| ATOM | 41 | NH2 | ARG | 5 | 21.864 | -10.790 | 19.307 | 1.00 | 21.29 | MTGL |
| ATOM | 42 | C | ARG | 5 | 24.390 | -7.238 | 24.009 | 1.00 | 16.18 | MTGL |
| ATOM | 43 | O | ARG | 5 | 24.869 | -8.311 | 23.642 | 1.00 | 16.58 | MTGL |
| ATOM | 44 | N | GLY | 6 | 24.853 | -6.577 | 25.064 | 1.00 | 16.16 | MTGL |
| ATOM | 45 | CA | GLY | 6 | 25.991 | -7.135 | 25.770 | 1.00 | 16.79 | MTGL |
| ATOM | 46 | C | GLY | 6 | 26.064 | -7.065 | 27.275 | 1.00 | 15.64 | MTGL |
| ATOM | 47 | O | GLY | 6 | 25.129 | -6.664 | 27.968 | 1.00 | 15.46 | MTGL |
| ATOM | 48 | N | VAL | 7 | 27.213 | -7.497 | 27.775 | 1.00 | 15.87 | MTGL |
| ATOM | 49 | CA | VAL | 7 | 27.491 | -7.500 | 29.199 | 1.00 | 15.12 | MTGL |
| ATOM | 50 | CB | VAL | 7 | 27.178 | -8.877 | 29.846 | 1.00 | 14.43 | MTGL |
| ATOM | 51 | CG1 | VAL | 7 | 25.750 | -9.293 | 29.537 | 1.00 | 12.85 | MTGL |
| ATOM | 52 | CG2 | VAL | 7 | 28.170 | -9.931 | 29.348 | 1.00 | 13.29 | MTGL |
| ATOM | 53 | C | VAL | 7 | 28.977 | -7.238 | 29.363 | 1.00 | 16.14 | MTGL |
| ATOM | 54 | O | VAL | 7 | 29.768 | -7.469 | 28.440 | 1.00 | 17.27 | MTGL |
| ATOM | 55 | N | ASP | 8 | 29.354 | -6.737 | 30.531 | 1.00 | 15.62 | MTGL |
| ATOM | 56 | CA | ASP | 8 | 30.755 | -6.514 | 30.842 | 1.00 | 15.20 | MTGL |
| ATOM | 57 | CB | ASP | 8 | 30.920 | -5.292 | 31.751 | 1.00 | 14.35 | MTGL |

Fig. 1

| ATOM | 58 | CG | ASP | 8 | 32.373 | -4.975 | 32.034 | 1.00 | 15.24 | MTGL |
|------|-----|-----|-----|----|--------|---------|--------|------|-------|------|
| ATOM | 59 | OD1 | ASP | 8 | 33.105 | -5.881 | 32.486 | 1.00 | 14.12 | MTGL |
| ATOM | 60 | OD2 | ASP | 8 | 32.784 | -3.817 | 31.805 | 1.00 | 14.89 | MTGL |
| ATOM | 61 | C | ASP | 8 | 31.108 | -7.793 | 31.602 | 1.00 | 14.33 | MTGL |
| ATOM | 62 | O | ASP | 8 | 30.573 | -8.040 | 32.683 | 1.00 | 15.61 | MTGL |
| ATOM | 63 | N | TRP | 9 | 31.980 | -8.614 | 31.027 | 1.00 | 13.27 | MTGL |
| ATOM | 64 | CA | TRP | 9 | 32.365 | -9.872 | 31.653 | 1.00 | 13.40 | MTGL |
| ATOM | 65 | CB | TRP | 9 | 32.124 | -11.020 | 30.663 | 1.00 | 12.58 | MTGL |
| ATOM | 66 | CG | TRP | 9 | 33.183 | -11.146 | 29.585 | 1.00 | 13.96 | MTGL |
| ATOM | 67 | CD2 | TRP | 9 | 33.682 | -12.362 | 29.012 | 1.00 | 13.39 | MTGL |
| ATOM | 68 | CE2 | TRP | 9 | 34.661 | -12.008 | 28.057 | 1.00 | 13.29 | MTGL |
| ATOM | 69 | CE3 | TRP | 9 | 33.396 | -13.719 | 29.214 | 1.00 | 14.51 | MTGL |
| ATOM | 70 | CD1 | TRP | 9 | 33.860 | -10.128 | 28.964 | 1.00 | 14.11 | MTGL |
| ATOM | 71 | NE1 | TRP | 9 | 34.752 | -10.640 | 28.046 | 1.00 | 13.31 | MTGL |
| ATOM | 72 | CZ2 | TRP | 9 | 35.357 | -12.964 | 27.305 | 1.00 | 14.73 | MTGL |
| ATOM | 73 | CZ3 | TRP | 9 | 34.093 | -14.673 | 28.463 | 1.00 | 14.84 | MTGL |
| ATOM | 74 | CH2 | TRP | 9 | 35.059 | -14.287 | 27.523 | 1.00 | 14.12 | MTGL |
| ATOM | 75 | C | TRP | 9 | 33.832 | -9.860 | 32.102 | 1.00 | 13.91 | MTGL |
| ATOM | 76 | O | TRP | 9 | 34.454 | -10.915 | 32.272 | 1.00 | 13.71 | MTGL |
| ATOM | 77 | N | SER | 10 | 34.373 | -8.660 | 32.295 | 1.00 | 13.08 | MTGL |
| ATOM | 78 | CA | SER | 10 | 35.770 | -8.481 | 32.692 | 1.00 | 14.15 | MTGL |
| ATOM | 79 | CB | SER | 10 | 35.983 | -7.052 | 33.193 | 1.00 | 13.75 | MTGL |
| ATOM | 80 | OG | SER | 10 | 35.691 | -6.114 | 32.168 | 1.00 | 14.07 | MTGL |
| ATOM | 81 | C | SER | 10 | 36.321 | -9.460 | 33.726 | 1.00 | 14.36 | MTGL |
| ATOM | 82 | O | SER | 10 | 37.414 | -9.994 | 33.553 | 1.00 | 14.45 | MTGL |
| ATOM | 83 | N | SER | 11 | 35.561 | -9.697 | 34.789 | 1.00 | 14.45 | MTGL |
| ATOM | 84 | CA | SER | 11 | 35.985 | -10.588 | 35.870 | 1.00 | 15.55 | MTGL |
| ATOM | 85 | CB | SER | 11 | 35.053 | -10.416 | 37.069 | 1.00 | 15.32 | MTGL |
| ATOM | 86 | OG | SER | 11 | 33.795 | -11.014 | 36.792 | 1.00 | 13.85 | MTGL |
| ATOM | 87 | C | SER | 11 | 36.043 | -12.080 | 35.544 | 1.00 | 16.02 | MTGL |
| ATOM | 88 | O | SER | 11 | 36.438 | -12.870 | 36.401 | 1.00 | 16.91 | MTGL |
| ATOM | 89 | N | VAL | 12 | 35.656 | -12.472 | 34.330 | 1.00 | 16.04 | MTGL |
| ATOM | 90 | CA | VAL | 12 | 35.640 | -13.890 | 33.969 | 1.00 | 14.89 | MTGL |
| ATOM | 91 | CB | VAL | 12 | 35.367 | -14.090 | 32.448 | 1.00 | 14.61 | MTGL |
| ATOM | 92 | CG1 | VAL | 12 | 36.418 | -13.371 | 31.604 | 1.00 | 13.79 | MTGL |
| ATOM | 93 | CG2 | VAL | 12 | 35.336 | -15.583 | 32.124 | 1.00 | 13.78 | MTGL |
| ATOM | 94 | C | VAL | 12 | 36.861 | -14.726 | 34.373 | 1.00 | 15.76 | MTGL |
| ATOM | 95 | O | VAL | 12 | 36.709 | -15.751 | 35.034 | 1.00 | 14.51 | MTGL |
| ATOM | 96 | N | VAL | 13 | 38.065 | -14.312 | 33.990 | 1.00 | 16.87 | MTGL |
| ATOM | 97 | CA | VAL | 13 | 39.246 | -15.100 | 34.343 | 1.00 | 17.35 | MTGL |
| ATOM | 98 | CB | VAL | 13 | 40.496 | -14.656 | 33.534 | 1.00 | 17.20 | MTGL |
| ATOM | 99 | CG1 | VAL | 13 | 41.775 | -15.198 | 34.177 | 1.00 | 16.12 | MTGL |
| ATOM | 100 | CG2 | VAL | 13 | 40.391 | -15.193 | 32.109 | 1.00 | 15.88 | MTGL |
| ATOM | 101 | C | VAL | 13 | 39.534 | -15.043 | 35.841 | 1.00 | 18.53 | MTGL |
| ATOM | 102 | O | VAL | 13 | 40.002 | -16.024 | 36.430 | 1.00 | 19.44 | MTGL |
| ATOM | 103 | N | VAL | 14 | 39.242 | -13.907 | 36.466 | 1.00 | 17.79 | MTGL |
| ATOM | 104 | CA | VAL | 14 | 39.463 | -13.785 | 37.900 | 1.00 | 18.35 | MTGL |
| ATOM | 105 | CB | VAL | 14 | 39.106 | -12.368 | 38.411 | 1.00 | 18.68 | MTGL |
| ATOM | 106 | CG1 | VAL | 14 | 39.117 | -12.347 | 39.939 | 1.00 | 19.58 | MTGL |
| ATOM | 107 | CG2 | VAL | 14 | 40.113 | -11.352 | 37.876 | 1.00 | 17.40 | MTGL |
| ATOM | 108 | C | VAL | 14 | 38.588 | -14.816 | 38.620 | 1.00 | 17.85 | MTGL |
| ATOM | 109 | O | VAL | 14 | 39.034 | -15.495 | 39.543 | 1.00 | 17.72 | MTGL |
| ATOM | 110 | N | GLU | 15 | 37.341 | -14.941 | 38.181 | 1.00 | 17.47 | MTGL |
| ATOM | 111 | CA | GLU | 15 | 36.420 | -15.889 | 38.800 | 1.00 | 18.52 | MTGL |
| ATOM | 112 | CB | GLU | 15 | 34.985 | -15.585 | 38.373 | 1.00 | 19.09 | MTGL |
| ATOM | 113 | CG | GLU | 15 | 34.392 | -14.361 | 39.056 | 1.00 | 20.86 | MTGL |
| ATOM | 114 | CD | GLU | 15 | 34.147 | -14.579 | 40.542 | 1.00 | 22.32 | MTGL |
| ATOM | 115 | OE1 | GLU | 15 | 35.113 | -14.887 | 41.273 | 1.00 | 23.29 | MTGL |

# Fig. 1 cont.

| ATOM | 116 | OE2 | GLU | 15 | 32.984 | -14.445 | 40.981 | 1.00 | 22.28 | MTGL |
| ATOM | 117 | C | GLU | 15 | 36.753 | -17.346 | 38.502 | 1.00 | 18.21 | MTGL |
| ATOM | 118 | O | GLU | 15 | 36.640 | -18.196 | 39.377 | 1.00 | 19.29 | MTGL |
| ATOM | 119 | N | GLU | 16 | 37.151 | -17.639 | 37.272 | 1.00 | 18.79 | MTGL |
| ATOM | 120 | CA | GLU | 16 | 37.504 | -19.006 | 36.921 | 1.00 | 19.07 | MTGL |
| ATOM | 121 | CB | GLU | 16 | 37.827 | -19.103 | 35.424 | 1.00 | 19.33 | MTGL |
| ATOM | 122 | CG | GLU | 16 | 36.645 | -18.735 | 34.530 | 1.00 | 19.54 | MTGL |
| ATOM | 123 | CD | GLU | 16 | 36.970 | -18.798 | 33.049 | 1.00 | 19.73 | MTGL |
| ATOM | 124 | OE1 | GLU | 16 | 38.143 | -18.577 | 32.683 | 1.00 | 19.62 | MTGL |
| ATOM | 125 | OE2 | GLU | 16 | 36.048 | -19.048 | 32.244 | 1.00 | 20.12 | MTGL |
| ATOM | 126 | C | GLU | 16 | 38.706 | -19.425 | 37.767 | 1.00 | 18.57 | MTGL |
| ATOM | 127 | O | GLU | 16 | 38.766 | -20.557 | 38.250 | 1.00 | 17.78 | MTGL |
| ATOM | 128 | N | ARG | 17 | 39.640 | -18.492 | 37.960 | 1.00 | 17.17 | MTGL |
| ATOM | 129 | CA | ARG | 17 | 40.842 | -18.759 | 38.756 | 1.00 | 18.26 | MTGL |
| ATOM | 130 | CB | ARG | 17 | 41.872 | -17.646 | 38.568 | 1.00 | 17.11 | MTGL |
| ATOM | 131 | CG | ARG | 17 | 42.593 | -17.719 | 37.240 | 1.00 | 16.83 | MTGL |
| ATOM | 132 | CD | ARG | 17 | 43.446 | -16.496 | 37.009 | 1.00 | 15.44 | MTGL |
| ATOM | 133 | NE | ARG | 17 | 44.246 | -16.636 | 35.801 | 1.00 | 15.36 | MTGL |
| ATOM | 134 | CZ | ARG | 17 | 45.084 | -15.708 | 35.357 | 1.00 | 15.76 | MTGL |
| ATOM | 135 | NH1 | ARG | 17 | 45.225 | -14.570 | 36.025 | 1.00 | 15.62 | MTGL |
| ATOM | 136 | NH2 | ARG | 17 | 45.788 | -15.922 | 34.254 | 1.00 | 15.66 | MTGL |
| ATOM | 137 | C | ARG | 17 | 40.502 | -18.887 | 40.225 | 1.00 | 18.97 | MTGL |
| ATOM | 138 | O | ARG | 17 | 41.279 | -19.407 | 41.017 | 1.00 | 19.60 | MTGL |
| ATOM | 139 | N | ALA | 18 | 39.330 | -18.396 | 40.590 | 1.00 | 19.85 | MTGL |
| ATOM | 140 | CA | ALA | 18 | 38.890 | -18.486 | 41.967 | 1.00 | 21.00 | MTGL |
| ATOM | 141 | CB | ALA | 18 | 38.071 | -17.262 | 42.339 | 1.00 | 21.45 | MTGL |
| ATOM | 142 | C | ALA | 18 | 38.066 | -19.756 | 42.154 | 1.00 | 21.18 | MTGL |
| ATOM | 143 | O | ALA | 18 | 37.495 | -19.982 | 43.216 | 1.00 | 21.53 | MTGL |
| ATOM | 144 | N | GLY | 19 | 37.994 | -20.577 | 41.110 | 1.00 | 20.78 | MTGL |
| ATOM | 145 | CA | GLY | 19 | 37.265 | -21.827 | 41.218 | 1.00 | 21.14 | MTGL |
| ATOM | 146 | C | GLY | 19 | 35.833 | -21.845 | 40.716 | 1.00 | 21.86 | MTGL |
| ATOM | 147 | O | GLY | 19 | 35.124 | -22.833 | 40.901 | 1.00 | 20.92 | MTGL |
| ATOM | 148 | N | VAL | 20 | 35.386 | -20.769 | 40.080 | 1.00 | 21.60 | MTGL |
| ATOM | 149 | CA | VAL | 20 | 34.021 | -20.755 | 39.578 | 1.00 | 21.91 | MTGL |
| ATOM | 150 | CB | VAL | 20 | 33.533 | -19.321 | 39.264 | 1.00 | 23.06 | MTGL |
| ATOM | 151 | CG1 | VAL | 20 | 32.126 | -19.370 | 38.674 | 1.00 | 22.39 | MTGL |
| ATOM | 152 | CG2 | VAL | 20 | 33.530 | -18.475 | 40.530 | 1.00 | 22.53 | MTGL |
| ATOM | 153 | C | VAL | 20 | 33.877 | -21.589 | 38.305 | 1.00 | 21.53 | MTGL |
| ATOM | 154 | O | VAL | 20 | 34.673 | -21.473 | 37.377 | 1.00 | 21.65 | MTGL |
| ATOM | 155 | N | SER | 21 | 32.864 | -22.444 | 38.283 | 0.50 | 21.24 | MTGL |
| ATOM | 156 | CA | SER | 21 | 32.596 | -23.272 | 37.116 | 0.50 | 21.35 | MTGL |
| ATOM | 157 | CB | SER | 21 | 32.602 | -24.757 | 37.488 | 0.50 | 22.01 | MTGL |
| ATOM | 158 | OG | SER | 21 | 33.897 | -25.165 | 37.901 | 0.50 | 22.69 | MTGL |
| ATOM | 159 | C | SER | 21 | 31.227 | -22.857 | 36.605 | 0.50 | 20.74 | MTGL |
| ATOM | 160 | O | SER | 21 | 30.205 | -23.167 | 37.214 | 0.50 | 20.32 | MTGL |
| ATOM | 161 | N | TYR | 22 | 31.216 | -22.134 | 35.491 | 1.00 | 20.34 | MTGL |
| ATOM | 162 | CA | TYR | 22 | 29.972 | -21.659 | 34.914 | 1.00 | 20.72 | MTGL |
| ATOM | 163 | CB | TYR | 22 | 30.270 | -20.511 | 33.952 | 1.00 | 19.18 | MTGL |
| ATOM | 164 | CG | TYR | 22 | 30.765 | -19.280 | 34.682 | 1.00 | 18.50 | MTGL |
| ATOM | 165 | CD1 | TYR | 22 | 29.909 | -18.548 | 35.503 | 1.00 | 17.85 | MTGL |
| ATOM | 166 | CE1 | TYR | 22 | 30.357 | -17.428 | 36.202 | 1.00 | 17.95 | MTGL |
| ATOM | 167 | CD2 | TYR | 22 | 32.092 | -18.865 | 34.578 | 1.00 | 17.87 | MTGL |
| ATOM | 168 | CE2 | TYR | 22 | 32.552 | -17.744 | 35.275 | 1.00 | 17.81 | MTGL |
| ATOM | 169 | CZ | TYR | 22 | 31.676 | -17.031 | 36.083 | 1.00 | 17.46 | MTGL |
| ATOM | 170 | OH | TYR | 22 | 32.107 | -15.915 | 36.767 | 1.00 | 17.47 | MTGL |
| ATOM | 171 | C | TYR | 22 | 29.152 | -22.742 | 34.239 | 1.00 | 21.41 | MTGL |
| ATOM | 172 | O | TYR | 22 | 29.688 | -23.634 | 33.588 | 1.00 | 21.91 | MTGL |
| ATOM | 173 | N | LYS | 23 | 27.839 | -22.654 | 34.414 | 1.00 | 22.66 | MTGL |

# Fig. 1 cont.

| ATOM | 174 | CA | LYS | 23 | 26.918 | -23.619 | 33.836 | 1.00 | 23.97 | MTGL |
|------|-----|-----|-----|-----|--------|---------|--------|------|-------|------|
| ATOM | 175 | CB | LYS | 23 | 26.387 | -24.537 | 34.936 | 1.00 | 24.47 | MTGL |
| ATOM | 176 | CG | LYS | 23 | 27.479 | -25.094 | 35.839 | 1.00 | 26.17 | MTGL |
| ATOM | 177 | CD | LYS | 23 | 26.894 | -25.778 | 37.066 | 1.00 | 28.12 | MTGL |
| ATOM | 178 | CE | LYS | 23 | 27.985 | -26.217 | 38.040 | 1.00 | 29.23 | MTGL |
| ATOM | 179 | NZ | LYS | 23 | 28.750 | -25.069 | 38.615 | 1.00 | 28.37 | MTGL |
| ATOM | 180 | C | LYS | 23 | 25.748 | -22.915 | 33.158 | 1.00 | 24.07 | MTGL |
| ATOM | 181 | O | LYS | 23 | 25.344 | -21.823 | 33.570 | 1.00 | 23.42 | MTGL |
| ATOM | 182 | N | ASN | 24 | 25.210 | -23.557 | 32.125 | 1.00 | 25.34 | MTGL |
| ATOM | 183 | CA | ASN | 24 | 24.074 | -23.020 | 31.390 | 1.00 | 26.76 | MTGL |
| ATOM | 184 | CB | ASN | 24 | 23.907 | -23.741 | 30.042 | 1.00 | 27.22 | MTGL |
| ATOM | 185 | CG | ASN | 24 | 23.925 | -25.258 | 30.174 | 1.00 | 28.00 | MTGL |
| ATOM | 186 | OD1 | ASN | 24 | 23.306 | -25.825 | 31.075 | 1.00 | 28.00 | MTGL |
| ATOM | 187 | ND2 | ASN | 24 | 24.626 | -25.923 | 29.258 | 1.00 | 28.41 | MTGL |
| ATOM | 188 | C | ASN | 24 | 22.802 | -23.171 | 32.216 | 1.00 | 27.53 | MTGL |
| ATOM | 189 | O | ASN | 24 | 22.830 | -23.727 | 33.315 | 1.00 | 26.87 | MTGL |
| ATOM | 190 | N | THR | 25 | 21.691 | -22.668 | 31.687 | 1.00 | 29.20 | MTGL |
| ATOM | 191 | CA | THR | 25 | 20.408 | -22.754 | 32.378 | 1.00 | 31.61 | MTGL |
| ATOM | 192 | CB | THR | 25 | 19.299 | -21.968 | 31.619 | 1.00 | 31.89 | MTGL |
| ATOM | 193 | OG1 | THR | 25 | 19.269 | -22.380 | 30.245 | 1.00 | 32.33 | MTGL |
| ATOM | 194 | CG2 | THR | 25 | 19.558 | -20.468 | 31.689 | 1.00 | 30.90 | MTGL |
| ATOM | 195 | C | THR | 25 | 19.968 | -24.209 | 32.540 | 1.00 | 33.20 | MTGL |
| ATOM | 196 | O | THR | 25 | 19.107 | -24.518 | 33.362 | 1.00 | 34.49 | MTGL |
| ATOM | 197 | N | ASN | 26 | 20.561 | -25.101 | 31.754 | 1.00 | 33.98 | MTGL |
| ATOM | 198 | CA | ASN | 26 | 20.229 | -26.521 | 31.831 | 1.00 | 34.91 | MTGL |
| ATOM | 199 | CB | ASN | 26 | 20.595 | -27.233 | 30.529 | 1.00 | 37.07 | MTGL |
| ATOM | 200 | CG | ASN | 26 | 19.515 | -27.114 | 29.479 | 1.00 | 38.98 | MTGL |
| ATOM | 201 | OD1 | ASN | 26 | 19.743 | -27.405 | 28.305 | 1.00 | 40.46 | MTGL |
| ATOM | 202 | ND2 | ASN | 26 | 18.325 | -26.696 | 29.898 | 1.00 | 39.01 | MTGL |
| ATOM | 203 | C | ASN | 26 | 21.000 | -27.153 | 32.967 | 1.00 | 33.95 | MTGL |
| ATOM | 204 | O | ASN | 26 | 20.752 | -28.294 | 33.356 | 1.00 | 34.07 | MTGL |
| ATOM | 205 | N | GLY | 27 | 21.952 | -26.402 | 33.493 | 1.00 | 32.34 | MTGL |
| ATOM | 206 | CA | GLY | 27 | 22.739 | -26.928 | 34.583 | 1.00 | 30.16 | MTGL |
| ATOM | 207 | C | GLY | 27 | 24.009 | -27.629 | 34.140 | 1.00 | 29.51 | MTGL |
| ATOM | 208 | O | GLY | 27 | 24.692 | -28.244 | 34.950 | 1.00 | 28.86 | MTGL |
| ATOM | 209 | N | ASN | 28 | 24.350 | -27.547 | 32.864 | 1.00 | 29.22 | MTGL |
| ATOM | 210 | CA | ASN | 28 | 25.565 | -28.205 | 32.419 | 1.00 | 28.62 | MTGL |
| ATOM | 211 | CB | ASN | 28 | 25.323 | -28.945 | 31.108 | 1.00 | 30.49 | MTGL |
| ATOM | 212 | CG | ASN | 28 | 24.313 | -30.063 | 31.258 | 1.00 | 31.94 | MTGL |
| ATOM | 213 | OD1 | ASN | 28 | 24.453 | -30.930 | 32.124 | 1.00 | 32.14 | MTGL |
| ATOM | 214 | ND2 | ASN | 28 | 23.288 | -30.049 | 30.417 | 1.00 | 32.11 | MTGL |
| ATOM | 215 | C | ASN | 28 | 26.714 | -27.228 | 32.264 | 1.00 | 27.80 | MTGL |
| ATOM | 216 | O | ASN | 28 | 26.537 | -26.085 | 31.831 | 1.00 | 26.86 | MTGL |
| ATOM | 217 | N | ALA | 29 | 27.897 | -27.695 | 32.629 | 1.00 | 26.54 | MTGL |
| ATOM | 218 | CA | ALA | 29 | 29.103 | -26.889 | 32.547 | 1.00 | 26.11 | MTGL |
| ATOM | 219 | CB | ALA | 29 | 30.290 | -27.687 | 33.067 | 1.00 | 25.81 | MTGL |
| ATOM | 220 | C | ALA | 29 | 29.351 | -26.456 | 31.110 | 1.00 | 25.11 | MTGL |
| ATOM | 221 | O | ALA | 29 | 29.232 | -27.254 | 30.184 | 1.00 | 24.31 | MTGL |
| ATOM | 222 | N | GLN | 30 | 29.713 | -25.192 | 30.932 | 1.00 | 23.82 | MTGL |
| ATOM | 223 | CA | GLN | 30 | 29.967 | -24.655 | 29.603 | 1.00 | 23.10 | MTGL |
| ATOM | 224 | CB | GLN | 30 | 28.620 | -24.424 | 28.901 | 1.00 | 23.68 | MTGL |
| ATOM | 225 | CG | GLN | 30 | 28.676 | -23.687 | 27.578 | 1.00 | 26.45 | MTGL |
| ATOM | 226 | CD | GLN | 30 | 27.335 | -23.695 | 26.858 | 1.00 | 27.43 | MTGL |
| ATOM | 227 | OE1 | GLN | 30 | 26.282 | -23.584 | 27.486 | 1.00 | 27.66 | MTGL |
| ATOM | 228 | NE2 | GLN | 30 | 27.371 | -23.815 | 25.537 | 1.00 | 27.00 | MTGL |
| ATOM | 229 | C | GLN | 30 | 30.748 | -23.350 | 29.740 | 1.00 | 21.50 | MTGL |
| ATOM | 230 | O | GLN | 30 | 30.556 | -22.609 | 30.700 | 1.00 | 21.61 | MTGL |
| ATOM | 231 | N | PRO | 31 | 31.661 | -23.066 | 28.797 | 1.00 | 20.08 | MTGL |

## Fig. 1 cont.

| ATOM | 232 | CD | PRO | 31 | 32.110 | -23.886 | 27.657 | 1.00 | 20.60 | MTGL |
|------|-----|-----|-----|----|--------|---------|--------|------|-------|------|
| ATOM | 233 | CA | PRO | 31 | 32.432 | -21.820 | 28.886 | 1.00 | 19.48 | MTGL |
| ATOM | 234 | CB | PRO | 31 | 33.262 | -21.834 | 27.603 | 1.00 | 20.47 | MTGL |
| ATOM | 235 | CG | PRO | 31 | 33.489 | -23.309 | 27.369 | 1.00 | 20.52 | MTGL |
| ATOM | 236 | C | PRO | 31 | 31.492 | -20.617 | 28.960 | 1.00 | 18.32 | MTGL |
| ATOM | 237 | O | PRO | 31 | 30.491 | -20.558 | 28.246 | 1.00 | 17.02 | MTGL |
| ATOM | 238 | N | LEU | 32 | 31.811 | -19.664 | 29.828 | 1.00 | 18.30 | MTGL |
| ATOM | 239 | CA | LEU | 32 | 30.971 | -18.477 | 29.987 | 1.00 | 18.52 | MTGL |
| ATOM | 240 | CB | LEU | 32 | 31.623 | -17.476 | 30.954 | 1.00 | 17.22 | MTGL |
| ATOM | 241 | CG | LEU | 32 | 30.828 | -16.190 | 31.227 | 1.00 | 17.71 | MTGL |
| ATOM | 242 | CD1 | LEU | 32 | 29.443 | -16.536 | 31.767 | 1.00 | 15.78 | MTGL |
| ATOM | 243 | CD2 | LEU | 32 | 31.588 | -15.319 | 32.235 | 1.00 | 15.40 | MTGL |
| ATOM | 244 | C | LEU | 32 | 30.655 | -17.776 | 28.669 | 1.00 | 17.46 | MTGL |
| ATOM | 245 | O | LEU | 32 | 29.504 | -17.413 | 28.429 | 1.00 | 18.85 | MTGL |
| ATOM | 246 | N | GLU | 33 | 31.660 | -17.581 | 27.818 | 1.00 | 16.99 | MTGL |
| ATOM | 247 | CA | GLU | 33 | 31.421 | -16.903 | 26.546 | 1.00 | 17.55 | MTGL |
| ATOM | 248 | CB | GLU | 33 | 32.716 | -16.763 | 25.735 | 1.00 | 17.22 | MTGL |
| ATOM | 249 | CG | GLU | 33 | 33.426 | -18.077 | 25.424 | 1.00 | 16.64 | MTGL |
| ATOM | 250 | CD | GLU | 33 | 34.496 | -18.417 | 26.453 | 1.00 | 16.72 | MTGL |
| ATOM | 251 | OE1 | GLU | 33 | 34.234 | -18.270 | 27.667 | 1.00 | 14.95 | MTGL |
| ATOM | 252 | OE2 | GLU | 33 | 35.597 | -18.840 | 26.048 | 1.00 | 16.02 | MTGL |
| ATOM | 253 | C | GLU | 33 | 30.369 | -17.630 | 25.712 | 1.00 | 18.39 | MTGL |
| ATOM | 254 | O | GLU | 33 | 29.576 | -16.988 | 25.021 | 1.00 | 19.97 | MTGL |
| ATOM | 255 | N | ASN | 34 | 30.354 | -18.959 | 25.779 | 1.00 | 18.00 | MTGL |
| ATOM | 256 | CA | ASN | 34 | 29.381 | -19.739 | 25.019 | 1.00 | 19.90 | MTGL |
| ATOM | 257 | CB | ASN | 34 | 29.793 | -21.214 | 24.955 | 1.00 | 21.66 | MTGL |
| ATOM | 258 | CG | ASN | 34 | 31.121 | -21.420 | 24.251 | 1.00 | 24.08 | MTGL |
| ATOM | 259 | OD1 | ASN | 34 | 31.355 | -20.886 | 23.168 | 1.00 | 25.77 | MTGL |
| ATOM | 260 | ND2 | ASN | 34 | 31.995 | -22.207 | 24.861 | 1.00 | 26.27 | MTGL |
| ATOM | 261 | C | ASN | 34 | 27.991 | -19.618 | 25.640 | 1.00 | 19.84 | MTGL |
| ATOM | 262 | O | ASN | 34 | 26.988 | -19.598 | 24.931 | 1.00 | 19.75 | MTGL |
| ATOM | 263 | N | ILE | 35 | 27.932 | -19.553 | 26.967 | 1.00 | 18.73 | MTGL |
| ATOM | 264 | CA | ILE | 35 | 26.656 | -19.404 | 27.656 | 1.00 | 18.63 | MTGL |
| ATOM | 265 | CB | ILE | 35 | 26.845 | -19.440 | 29.188 | 1.00 | 18.28 | MTGL |
| ATOM | 266 | CG2 | ILE | 35 | 25.556 | -19.028 | 29.890 | 1.00 | 17.35 | MTGL |
| ATOM | 267 | CG1 | ILE | 35 | 27.270 | -20.844 | 29.623 | 1.00 | 18.06 | MTGL |
| ATOM | 268 | CD1 | ILE | 35 | 27.652 | -20.946 | 31.091 | 1.00 | 19.14 | MTGL |
| ATOM | 269 | C | ILE | 35 | 26.048 | -18.053 | 27.258 | 1.00 | 18.92 | MTGL |
| ATOM | 270 | O | ILE | 35 | 24.867 | -17.966 | 26.907 | 1.00 | 18.51 | MTGL |
| ATOM | 271 | N | LEU | 36 | 26.866 | -17.005 | 27.313 | 1.00 | 18.03 | MTGL |
| ATOM | 272 | CA | LEU | 36 | 26.416 | -15.665 | 26.956 | 1.00 | 17.16 | MTGL |
| ATOM | 273 | CB | LEU | 36 | 27.563 | -14.660 | 27.110 | 1.00 | 17.06 | MTGL |
| ATOM | 274 | CG | LEU | 36 | 28.076 | -14.411 | 28.538 | 1.00 | 16.94 | MTGL |
| ATOM | 275 | CD1 | LEU | 36 | 29.323 | -13.516 | 28.504 | 1.00 | 14.36 | MTGL |
| ATOM | 276 | CD2 | LEU | 36 | 26.969 | -13.761 | 29.372 | 1.00 | 16.43 | MTGL |
| ATOM | 277 | C | LEU | 36 | 25.891 | -15.636 | 25.522 | 1.00 | 17.26 | MTGL |
| ATOM | 278 | O | LEU | 36 | 24.795 | -15.132 | 25.270 | 1.00 | 16.08 | MTGL |
| ATOM | 279 | N | ALA | 37 | 26.675 | -16.174 | 24.589 | 1.00 | 17.12 | MTGL |
| ATOM | 280 | CA | ALA | 37 | 26.278 | -16.203 | 23.187 | 1.00 | 17.86 | MTGL |
| ATOM | 281 | CB | ALA | 37 | 27.362 | -16.863 | 22.338 | 1.00 | 16.93 | MTGL |
| ATOM | 282 | C | ALA | 37 | 24.961 | -16.948 | 23.014 | 1.00 | 18.20 | MTGL |
| ATOM | 283 | O | ALA | 37 | 24.062 | -16.480 | 22.314 | 1.00 | 19.46 | MTGL |
| ATOM | 284 | N | ALA | 38 | 24.850 | -18.105 | 23.658 | 1.00 | 18.38 | MTGL |
| ATOM | 285 | CA | ALA | 38 | 23.643 | -18.917 | 23.560 | 1.00 | 20.05 | MTGL |
| ATOM | 286 | CB | ALA | 38 | 23.809 | -20.212 | 24.358 | 1.00 | 19.05 | MTGL |
| ATOM | 287 | C | ALA | 38 | 22.419 | -18.154 | 24.049 | 1.00 | 20.48 | MTGL |
| ATOM | 288 | O | ALA | 38 | 21.294 | -18.447 | 23.634 | 1.00 | 21.25 | MTGL |
| ATOM | 289 | N | ASN | 39 | 22.637 | -17.173 | 24.923 | 1.00 | 20.10 | MTGL |

Fig. 1 cont.

| ATOM | 290 | CA | ASN | 39 | 21.531 | −16.390 | 25.460 | 1.00 | 19.15 | MTGL |
|------|-----|-----|-----|-----|--------|---------|--------|------|-------|------|
| ATOM | 291 | CB | ASN | 39 | 21.717 | −16.168 | 26.963 | 1.00 | 19.77 | MTGL |
| ATOM | 292 | CG | ASN | 39 | 21.416 | −17.414 | 27.774 | 1.00 | 19.60 | MTGL |
| ATOM | 293 | OD1 | ASN | 39 | 22.241 | −18.327 | 27.872 | 1.00 | 22.00 | MTGL |
| ATOM | 294 | ND2 | ASN | 39 | 20.224 | −17.467 | 28.346 | 1.00 | 18.25 | MTGL |
| ATOM | 295 | C | ASN | 39 | 21.253 | −15.056 | 24.768 | 1.00 | 18.64 | MTGL |
| ATOM | 296 | O | ASN | 39 | 20.544 | −14.213 | 25.317 | 1.00 | 19.42 | MTGL |
| ATOM | 297 | N | GLY | 40 | 21.803 | −14.862 | 23.572 | 1.00 | 17.47 | MTGL |
| ATOM | 298 | CA | GLY | 40 | 21.535 | −13.635 | 22.837 | 1.00 | 17.26 | MTGL |
| ATOM | 299 | C | GLY | 40 | 22.585 | −12.537 | 22.880 | 1.00 | 17.22 | MTGL |
| ATOM | 300 | O | GLY | 40 | 22.523 | −11.594 | 22.095 | 1.00 | 17.12 | MTGL |
| ATOM | 301 | N | VAL | 41 | 23.544 | −12.641 | 23.791 | 1.00 | 16.80 | MTGL |
| ATOM | 302 | CA | VAL | 41 | 24.589 | −11.631 | 23.893 | 1.00 | 15.92 | MTGL |
| ATOM | 303 | CB | VAL | 41 | 25.510 | −11.908 | 25.103 | 1.00 | 16.19 | MTGL |
| ATOM | 304 | CG1 | VAL | 41 | 26.630 | −10.888 | 25.144 | 1.00 | 14.75 | MTGL |
| ATOM | 305 | CG2 | VAL | 41 | 24.707 | −11.875 | 26.397 | 1.00 | 15.59 | MTGL |
| ATOM | 306 | C | VAL | 41 | 25.441 | −11.645 | 22.626 | 1.00 | 15.77 | MTGL |
| ATOM | 307 | O | VAL | 41 | 25.832 | −12.715 | 22.158 | 1.00 | 14.76 | MTGL |
| ATOM | 308 | N | ASN | 42 | 25.724 | −10.469 | 22.064 | 1.00 | 16.34 | MTGL |
| ATOM | 309 | CA | ASN | 42 | 26.559 | −10.406 | 20.864 | 1.00 | 16.57 | MTGL |
| ATOM | 310 | CB | ASN | 42 | 25.771 | −9.889 | 19.646 | 1.00 | 17.06 | MTGL |
| ATOM | 311 | CG | ASN | 42 | 25.299 | −8.443 | 19.798 | 1.00 | 18.15 | MTGL |
| ATOM | 312 | OD1 | ASN | 42 | 25.727 | −7.709 | 20.694 | 1.00 | 18.63 | MTGL |
| ATOM | 313 | ND2 | ASN | 42 | 24.416 | −8.028 | 18.898 | 1.00 | 16.75 | MTGL |
| ATOM | 314 | C | ASN | 42 | 27.812 | −9.560 | 21.048 | 1.00 | 16.81 | MTGL |
| ATOM | 315 | O | ASN | 42 | 28.651 | −9.478 | 20.147 | 1.00 | 17.52 | MTGL |
| ATOM | 316 | N | THR | 43 | 27.952 | −8.951 | 22.221 | 1.00 | 16.55 | MTGL |
| ATOM | 317 | CA | THR | 43 | 29.108 | −8.108 | 22.502 | 1.00 | 15.96 | MTGL |
| ATOM | 318 | CB | THR | 43 | 28.827 | −6.634 | 22.136 | 1.00 | 16.50 | MTGL |
| ATOM | 319 | OG1 | THR | 43 | 28.192 | −6.565 | 20.850 | 1.00 | 17.26 | MTGL |
| ATOM | 320 | CG2 | THR | 43 | 30.123 | −5.840 | 22.102 | 1.00 | 15.22 | MTGL |
| ATOM | 321 | C | THR | 43 | 29.487 | −8.144 | 23.976 | 1.00 | 15.93 | MTGL |
| ATOM | 322 | O | THR | 43 | 28.618 | −8.180 | 24.849 | 1.00 | 16.10 | MTGL |
| ATOM | 323 | N | VAL | 44 | 30.786 | −8.148 | 24.251 | 1.00 | 14.74 | MTGL |
| ATOM | 324 | CA | VAL | 44 | 31.251 | −8.136 | 25.626 | 1.00 | 15.41 | MTGL |
| ATOM | 325 | CB | VAL | 44 | 32.038 | −9.418 | 26.012 | 1.00 | 16.13 | MTGL |
| ATOM | 326 | CG1 | VAL | 44 | 31.084 | −10.603 | 26.096 | 1.00 | 16.11 | MTGL |
| ATOM | 327 | CG2 | VAL | 44 | 33.146 | −9.689 | 25.004 | 1.00 | 14.58 | MTGL |
| ATOM | 328 | C | VAL | 44 | 32.137 | −6.922 | 25.849 | 1.00 | 15.69 | MTGL |
| ATOM | 329 | O | VAL | 44 | 32.974 | −6.574 | 25.014 | 1.00 | 16.22 | MTGL |
| ATOM | 330 | N | ARG | 45 | 31.916 | −6.271 | 26.981 | 1.00 | 14.86 | MTGL |
| ATOM | 331 | CA | ARG | 45 | 32.662 | −5.091 | 27.383 | 1.00 | 15.51 | MTGL |
| ATOM | 332 | CB | ARG | 45 | 31.702 | −4.129 | 28.087 | 1.00 | 16.51 | MTGL |
| ATOM | 333 | CG | ARG | 45 | 32.297 | −2.828 | 28.597 | 1.00 | 17.41 | MTGL |
| ATOM | 334 | CD | ARG | 45 | 31.143 | −1.971 | 29.107 | 1.00 | 18.63 | MTGL |
| ATOM | 335 | NE | ARG | 45 | 31.519 | −0.636 | 29.554 | 1.00 | 19.44 | MTGL |
| ATOM | 336 | CZ | ARG | 45 | 31.756 | −0.309 | 30.820 | 1.00 | 19.56 | MTGL |
| ATOM | 337 | NH1 | ARG | 45 | 31.671 | −1.225 | 31.777 | 1.00 | 18.15 | MTGL |
| ATOM | 338 | NH2 | ARG | 45 | 32.032 | 0.949 | 31.130 | 1.00 | 19.68 | MTGL |
| ATOM | 339 | C | ARG | 45 | 33.752 | −5.561 | 28.342 | 1.00 | 15.10 | MTGL |
| ATOM | 340 | O | ARG | 45 | 33.516 | −6.446 | 29.168 | 1.00 | 13.85 | MTGL |
| ATOM | 341 | N | GLN | 46 | 34.938 | −4.965 | 28.232 | 1.00 | 14.87 | MTGL |
| ATOM | 342 | CA | GLN | 46 | 36.071 | −5.331 | 29.074 | 1.00 | 14.52 | MTGL |
| ATOM | 343 | CB | GLN | 46 | 37.030 | −6.246 | 28.296 | 1.00 | 14.23 | MTGL |
| ATOM | 344 | CG | GLN | 46 | 36.376 | −7.512 | 27.746 | 1.00 | 14.12 | MTGL |
| ATOM | 345 | CD | GLN | 46 | 37.310 | −8.358 | 26.902 | 1.00 | 13.86 | MTGL |
| ATOM | 346 | OE1 | GLN | 46 | 36.895 | −9.363 | 26.335 | 1.00 | 15.22 | MTGL |
| ATOM | 347 | NE2 | GLN | 46 | 38.575 | −7.958 | 26.814 | 1.00 | 13.21 | MTGL |

# Fig. 1 cont.

| ATOM | 348 | C   | GLN | 46 | 36.831 | -4.089 | 29.534 | 1.00 | 15.79 | MTGL |
|------|-----|-----|-----|----|--------|--------|--------|------|-------|------|
| ATOM | 349 | O   | GLN | 46 | 37.153 | -3.211 | 28.728 | 1.00 | 15.74 | MTGL |
| ATOM | 350 | N   | ARG | 47 | 37.111 | -4.005 | 30.830 | 1.00 | 15.01 | MTGL |
| ATOM | 351 | CA  | ARG | 47 | 37.851 | -2.866 | 31.350 | 1.00 | 15.05 | MTGL |
| ATOM | 352 | CB  | ARG | 47 | 37.524 | -2.631 | 32.828 | 1.00 | 13.91 | MTGL |
| ATOM | 353 | CG  | ARG | 47 | 37.649 | -3.868 | 33.710 | 1.00 | 13.56 | MTGL |
| ATOM | 354 | CD  | ARG | 47 | 37.391 | -3.520 | 35.175 | 1.00 | 13.26 | MTGL |
| ATOM | 355 | NE  | ARG | 47 | 37.207 | -4.710 | 36.004 | 1.00 | 12.49 | MTGL |
| ATOM | 356 | CZ  | ARG | 47 | 36.063 | -5.382 | 36.117 | 1.00 | 13.71 | MTGL |
| ATOM | 357 | NH1 | ARG | 47 | 34.983 | -4.981 | 35.457 | 1.00 | 13.79 | MTGL |
| ATOM | 358 | NH2 | ARG | 47 | 36.004 | -6.477 | 36.876 | 1.00 | 12.61 | MTGL |
| ATOM | 359 | C   | ARG | 47 | 39.347 | -3.107 | 31.182 | 1.00 | 15.50 | MTGL |
| ATOM | 360 | O   | ARG | 47 | 39.849 | -4.209 | 31.433 | 1.00 | 15.21 | MTGL |
| ATOM | 361 | N   | VAL | 48 | 40.056 | -2.072 | 30.745 | 1.00 | 15.84 | MTGL |
| ATOM | 362 | CA  | VAL | 48 | 41.496 | -2.171 | 30.557 | 1.00 | 15.53 | MTGL |
| ATOM | 363 | CB  | VAL | 48 | 41.899 | -1.874 | 29.102 | 1.00 | 16.38 | MTGL |
| ATOM | 364 | CG1 | VAL | 48 | 43.418 | -1.906 | 28.975 | 1.00 | 15.45 | MTGL |
| ATOM | 365 | CG2 | VAL | 48 | 41.258 | -2.892 | 28.160 | 1.00 | 14.39 | MTGL |
| ATOM | 366 | C   | VAL | 48 | 42.222 | -1.185 | 31.459 | 1.00 | 16.31 | MTGL |
| ATOM | 367 | O   | VAL | 48 | 41.941 | 0.013  | 31.433 | 1.00 | 14.76 | MTGL |
| ATOM | 368 | N   | TRP | 49 | 43.139 | -1.707 | 32.270 | 1.00 | 16.64 | MTGL |
| ATOM | 369 | CA  | TRP | 49 | 43.938 | -0.890 | 33.172 | 1.00 | 17.13 | MTGL |
| ATOM | 370 | CB  | TRP | 49 | 43.893 | -1.458 | 34.598 | 1.00 | 17.19 | MTGL |
| ATOM | 371 | CG  | TRP | 49 | 42.525 | -1.365 | 35.239 | 1.00 | 17.50 | MTGL |
| ATOM | 372 | CD2 | TRP | 49 | 42.129 | -1.903 | 36.510 | 1.00 | 17.36 | MTGL |
| ATOM | 373 | CE2 | TRP | 49 | 40.773 | -1.550 | 36.710 | 1.00 | 17.08 | MTGL |
| ATOM | 374 | CE3 | TRP | 49 | 42.786 | -2.651 | 37.497 | 1.00 | 16.24 | MTGL |
| ATOM | 375 | CD1 | TRP | 49 | 41.426 | -0.728 | 34.736 | 1.00 | 17.53 | MTGL |
| ATOM | 376 | NE1 | TRP | 49 | 40.370 | -0.832 | 35.614 | 1.00 | 17.76 | MTGL |
| ATOM | 377 | CZ2 | TRP | 49 | 40.063 | -1.915 | 37.860 | 1.00 | 16.34 | MTGL |
| ATOM | 378 | CZ3 | TRP | 49 | 42.079 | -3.014 | 38.642 | 1.00 | 17.30 | MTGL |
| ATOM | 379 | CH2 | TRP | 49 | 40.729 | -2.645 | 38.812 | 1.00 | 16.66 | MTGL |
| ATOM | 380 | C   | TRP | 49 | 45.369 | -0.870 | 32.632 | 1.00 | 17.96 | MTGL |
| ATOM | 381 | O   | TRP | 49 | 45.819 | -1.830 | 32.007 | 1.00 | 16.92 | MTGL |
| ATOM | 382 | N   | VAL | 50 | 46.078 | 0.228  | 32.874 | 1.00 | 18.74 | MTGL |
| ATOM | 383 | CA  | VAL | 50 | 47.438 | 0.408  | 32.373 | 1.00 | 18.43 | MTGL |
| ATOM | 384 | CB  | VAL | 50 | 47.898 | 1.865  | 32.604 | 1.00 | 17.51 | MTGL |
| ATOM | 385 | CG1 | VAL | 50 | 49.310 | 2.061  | 32.069 | 1.00 | 16.69 | MTGL |
| ATOM | 386 | CG2 | VAL | 50 | 46.931 | 2.814  | 31.912 | 1.00 | 16.38 | MTGL |
| ATOM | 387 | C   | VAL | 50 | 48.492 | -0.568 | 32.910 | 1.00 | 20.17 | MTGL |
| ATOM | 388 | O   | VAL | 50 | 49.035 | -1.359 | 32.141 | 1.00 | 20.17 | MTGL |
| ATOM | 389 | N   | ASN | 51 | 48.809 | -0.513 | 34.203 | 1.00 | 20.54 | MTGL |
| ATOM | 390 | CA  | ASN | 51 | 49.800 | -1.438 | 34.780 | 1.00 | 22.14 | MTGL |
| ATOM | 391 | CB  | ASN | 51 | 51.181 | -0.778 | 34.894 | 1.00 | 22.82 | MTGL |
| ATOM | 392 | CG  | ASN | 51 | 51.899 | -0.671 | 33.564 | 1.00 | 24.64 | MTGL |
| ATOM | 393 | OD1 | ASN | 51 | 52.211 | 0.430  | 33.102 | 1.00 | 25.29 | MTGL |
| ATOM | 394 | ND2 | ASN | 51 | 52.180 | -1.813 | 32.945 | 1.00 | 24.48 | MTGL |
| ATOM | 395 | C   | ASN | 51 | 49.416 | -1.943 | 36.173 | 1.00 | 22.18 | MTGL |
| ATOM | 396 | O   | ASN | 51 | 50.177 | -1.771 | 37.119 | 1.00 | 23.10 | MTGL |
| ATOM | 397 | N   | PRO | 52 | 48.242 | -2.584 | 36.317 | 1.00 | 21.49 | MTGL |
| ATOM | 398 | CD  | PRO | 52 | 47.333 | -3.089 | 35.273 | 1.00 | 20.91 | MTGL |
| ATOM | 399 | CA  | PRO | 52 | 47.847 | -3.079 | 37.642 | 1.00 | 20.88 | MTGL |
| ATOM | 400 | CB  | PRO | 52 | 46.509 | -3.769 | 37.370 | 1.00 | 20.37 | MTGL |
| ATOM | 401 | CG  | PRO | 52 | 46.683 | -4.283 | 35.963 | 1.00 | 20.56 | MTGL |
| ATOM | 402 | C   | PRO | 52 | 48.905 | -4.041 | 38.177 | 1.00 | 21.68 | MTGL |
| ATOM | 403 | O   | PRO | 52 | 49.390 | -4.902 | 37.449 | 1.00 | 20.78 | MTGL |
| ATOM | 404 | N   | ALA | 53 | 49.261 | -3.891 | 39.448 | 1.00 | 22.20 | MTGL |
| ATOM | 405 | CA  | ALA | 53 | 50.278 | -4.739 | 40.061 | 1.00 | 23.49 | MTGL |

Fig. 1 cont.

| ATOM | 406 | CB | ALA | 53 | 50.409 | -4.407 | 41.549 | 1.00 | 23.83 | MTGL |
|------|-----|-----|-----|-----|--------|--------|--------|------|-------|------|
| ATOM | 407 | C | ALA | 53 | 50.037 | -6.235 | 39.883 | 1.00 | 23.68 | MTGL |
| ATOM | 408 | O | ALA | 53 | 50.937 | -6.960 | 39.466 | 1.00 | 23.33 | MTGL |
| ATOM | 409 | N | ASP | 54 | 48.831 | -6.704 | 40.195 | 1.00 | 24.06 | MTGL |
| ATOM | 410 | CA | ASP | 54 | 48.539 | -8.126 | 40.058 | 1.00 | 24.64 | MTGL |
| ATOM | 411 | CB | ASP | 54 | 47.400 | -8.540 | 40.994 | 1.00 | 26.42 | MTGL |
| ATOM | 412 | CG | ASP | 54 | 46.109 | -7.805 | 40.706 | 1.00 | 27.54 | MTGL |
| ATOM | 413 | OD1 | ASP | 54 | 45.834 | -7.515 | 39.522 | 1.00 | 29.32 | MTGL |
| ATOM | 414 | OD2 | ASP | 54 | 45.360 | -7.529 | 41.664 | 1.00 | 27.59 | MTGL |
| ATOM | 415 | C | ASP | 54 | 48.207 | -8.560 | 38.631 | 1.00 | 24.00 | MTGL |
| ATOM | 416 | O | ASP | 54 | 47.878 | -9.720 | 38.396 | 1.00 | 24.44 | MTGL |
| ATOM | 417 | N | GLY | 55 | 48.286 | -7.630 | 37.686 | 1.00 | 22.74 | MTGL |
| ATOM | 418 | CA | GLY | 55 | 48.013 | -7.959 | 36.296 | 1.00 | 21.74 | MTGL |
| ATOM | 419 | C | GLY | 55 | 46.566 | -8.102 | 35.854 | 1.00 | 20.84 | MTGL |
| ATOM | 420 | O | GLY | 55 | 46.294 | -8.150 | 34.652 | 1.00 | 20.70 | MTGL |
| ATOM | 421 | N | ASN | 56 | 45.627 | -8.173 | 36.791 | 1.00 | 20.23 | MTGL |
| ATOM | 422 | CA | ASN | 56 | 44.229 | -8.320 | 36.399 | 1.00 | 19.77 | MTGL |
| ATOM | 423 | CB | ASN | 56 | 43.329 | -8.530 | 37.623 | 1.00 | 21.09 | MTGL |
| ATOM | 424 | CG | ASN | 56 | 43.569 | -9.876 | 38.301 | 1.00 | 22.81 | MTGL |
| ATOM | 425 | OD1 | ASN | 56 | 43.921 | -10.859 | 37.647 | 1.00 | 20.74 | MTGL |
| ATOM | 426 | ND2 | ASN | 56 | 43.359 | -9.926 | 39.611 | 1.00 | 22.17 | MTGL |
| ATOM | 427 | C | ASN | 56 | 43.751 | -7.108 | 35.612 | 1.00 | 18.30 | MTGL |
| ATOM | 428 | O | ASN | 56 | 43.972 | -5.968 | 36.016 | 1.00 | 17.82 | MTGL |
| ATOM | 429 | N | TYR | 57 | 43.108 | -7.376 | 34.480 | 1.00 | 16.29 | MTGL |
| ATOM | 430 | CA | TYR | 57 | 42.570 | -6.353 | 33.591 | 1.00 | 15.51 | MTGL |
| ATOM | 431 | CB | TYR | 57 | 41.680 | -5.376 | 34.368 | 1.00 | 15.50 | MTGL |
| ATOM | 432 | CG | TYR | 57 | 40.756 | -6.062 | 35.348 | 1.00 | 16.25 | MTGL |
| ATOM | 433 | CD1 | TYR | 57 | 39.969 | -7.150 | 34.955 | 1.00 | 15.93 | MTGL |
| ATOM | 434 | CE1 | TYR | 57 | 39.137 | -7.799 | 35.859 | 1.00 | 16.29 | MTGL |
| ATOM | 435 | CD2 | TYR | 57 | 40.681 | -5.642 | 36.671 | 1.00 | 16.32 | MTGL |
| ATOM | 436 | CE2 | TYR | 57 | 39.847 | -6.288 | 37.585 | 1.00 | 17.00 | MTGL |
| ATOM | 437 | CZ | TYR | 57 | 39.080 | -7.363 | 37.172 | 1.00 | 15.31 | MTGL |
| ATOM | 438 | OH | TYR | 57 | 38.254 | -8.000 | 38.066 | 1.00 | 15.12 | MTGL |
| ATOM | 439 | C | TYR | 57 | 43.627 | -5.579 | 32.807 | 1.00 | 15.53 | MTGL |
| ATOM | 440 | O | TYR | 57 | 43.315 | -4.561 | 32.189 | 1.00 | 14.98 | MTGL |
| ATOM | 441 | N | ASN | 58 | 44.877 | -6.033 | 32.825 | 1.00 | 14.46 | MTGL |
| ATOM | 442 | CA | ASN | 58 | 45.876 | -5.327 | 32.032 | 1.00 | 15.65 | MTGL |
| ATOM | 443 | CB | ASN | 58 | 47.314 | -5.594 | 32.522 | 1.00 | 15.44 | MTGL |
| ATOM | 444 | CG | ASN | 58 | 47.783 | -7.030 | 32.319 | 1.00 | 16.49 | MTGL |
| ATOM | 445 | OD1 | ASN | 58 | 48.869 | -7.390 | 32.779 | 1.00 | 18.71 | MTGL |
| ATOM | 446 | ND2 | ASN | 58 | 46.995 | -7.844 | 31.640 | 1.00 | 13.70 | MTGL |
| ATOM | 447 | C | ASN | 58 | 45.660 | -5.763 | 30.582 | 1.00 | 16.00 | MTGL |
| ATOM | 448 | O | ASN | 58 | 44.774 | -6.579 | 30.317 | 1.00 | 14.12 | MTGL |
| ATOM | 449 | N | LEU | 59 | 46.447 | -5.235 | 29.649 | 1.00 | 16.39 | MTGL |
| ATOM | 450 | CA | LEU | 59 | 46.241 | -5.564 | 28.242 | 1.00 | 17.31 | MTGL |
| ATOM | 451 | CB | LEU | 59 | 47.192 | -4.751 | 27.356 | 1.00 | 17.07 | MTGL |
| ATOM | 452 | CG | LEU | 59 | 46.797 | -4.743 | 25.874 | 1.00 | 17.21 | MTGL |
| ATOM | 453 | CD1 | LEU | 59 | 45.367 | -4.208 | 25.722 | 1.00 | 16.29 | MTGL |
| ATOM | 454 | CD2 | LEU | 59 | 47.769 | -3.882 | 25.085 | 1.00 | 16.17 | MTGL |
| ATOM | 455 | C | LEU | 59 | 46.333 | -7.046 | 27.880 | 1.00 | 17.51 | MTGL |
| ATOM | 456 | O | LEU | 59 | 45.517 | -7.537 | 27.096 | 1.00 | 17.20 | MTGL |
| ATOM | 457 | N | ASP | 60 | 47.317 | -7.754 | 28.432 | 1.00 | 17.48 | MTGL |
| ATOM | 458 | CA | ASP | 60 | 47.460 | -9.183 | 28.152 | 1.00 | 18.05 | MTGL |
| ATOM | 459 | CB | ASP | 60 | 48.700 | -9.768 | 28.837 | 1.00 | 20.82 | MTGL |
| ATOM | 460 | CG | ASP | 60 | 49.995 | -9.286 | 28.217 | 1.00 | 23.01 | MTGL |
| ATOM | 461 | OD1 | ASP | 60 | 50.012 | -9.009 | 26.999 | 1.00 | 25.11 | MTGL |
| ATOM | 462 | OD2 | ASP | 60 | 51.002 | -9.204 | 28.946 | 1.00 | 25.50 | MTGL |
| ATOM | 463 | C | ASP | 60 | 46.237 | -9.943 | 28.647 | 1.00 | 17.40 | MTGL |

Fig. 1 cont.

| ATOM | 464 | O   | ASP | 60 | 45.749 | -10.856 | 27.984 | 1.00 | 16.59 | MTGL |
|------|-----|-----|-----|----|--------|---------|--------|------|-------|------|
| ATOM | 465 | N   | TYR | 61 | 45.756 | -9.573  | 29.827 | 1.00 | 15.42 | MTGL |
| ATOM | 466 | CA  | TYR | 61 | 44.580 | -10.215 | 30.398 | 1.00 | 15.67 | MTGL |
| ATOM | 467 | CB  | TYR | 61 | 44.266 | -9.581  | 31.759 | 1.00 | 15.24 | MTGL |
| ATOM | 468 | CG  | TYR | 61 | 43.000 | -10.071 | 32.427 | 1.00 | 15.21 | MTGL |
| ATOM | 469 | CD1 | TYR | 61 | 41.746 | -9.597  | 32.032 | 1.00 | 15.96 | MTGL |
| ATOM | 470 | CE1 | TYR | 61 | 40.578 | -10.025 | 32.670 | 1.00 | 14.87 | MTGL |
| ATOM | 471 | CD2 | TYR | 61 | 43.058 | -10.990 | 33.473 | 1.00 | 15.54 | MTGL |
| ATOM | 472 | CE2 | TYR | 61 | 41.899 | -11.428 | 34.120 | 1.00 | 14.46 | MTGL |
| ATOM | 473 | CZ  | TYR | 61 | 40.662 | -10.943 | 33.714 | 1.00 | 16.75 | MTGL |
| ATOM | 474 | OH  | TYR | 61 | 39.511 | -11.379 | 34.345 | 1.00 | 14.25 | MTGL |
| ATOM | 475 | C   | TYR | 61 | 43.400 | -10.042 | 29.434 | 1.00 | 15.36 | MTGL |
| ATOM | 476 | O   | TYR | 61 | 42.651 | -10.987 | 29.175 | 1.00 | 15.76 | MTGL |
| ATOM | 477 | N   | ASN | 62 | 43.257 | -8.834  | 28.897 | 1.00 | 14.42 | MTGL |
| ATOM | 478 | CA  | ASN | 62 | 42.174 | -8.509  | 27.971 | 1.00 | 16.00 | MTGL |
| ATOM | 479 | CB  | ASN | 62 | 42.072 | -6.990  | 27.811 | 1.00 | 15.99 | MTGL |
| ATOM | 480 | CG  | ASN | 62 | 41.231 | -6.354  | 28.895 | 1.00 | 18.27 | MTGL |
| ATOM | 481 | OD1 | ASN | 62 | 39.998 | -6.396  | 28.840 | 1.00 | 18.23 | MTGL |
| ATOM | 482 | ND2 | ASN | 62 | 41.887 | -5.780  | 29.901 | 1.00 | 16.02 | MTGL |
| ATOM | 483 | C   | ASN | 62 | 42.306 | -9.172  | 26.600 | 1.00 | 16.04 | MTGL |
| ATOM | 484 | O   | ASN | 62 | 41.306 | -9.546  | 25.990 | 1.00 | 15.56 | MTGL |
| ATOM | 485 | N   | ILE | 63 | 43.534 | -9.311  | 26.110 | 1.00 | 16.06 | MTGL |
| ATOM | 486 | CA  | ILE | 63 | 43.732 | -9.952  | 24.824 | 1.00 | 17.20 | MTGL |
| ATOM | 487 | CB  | ILE | 63 | 45.202 | -9.827  | 24.350 | 1.00 | 16.83 | MTGL |
| ATOM | 488 | CG2 | ILE | 63 | 45.481 | -10.814 | 23.214 | 1.00 | 17.67 | MTGL |
| ATOM | 489 | CG1 | ILE | 63 | 45.463 | -8.391  | 23.887 | 1.00 | 17.41 | MTGL |
| ATOM | 490 | CD1 | ILE | 63 | 46.910 | -8.105  | 23.521 | 1.00 | 18.09 | MTGL |
| ATOM | 491 | C   | ILE | 63 | 43.333 | -11.420 | 24.945 | 1.00 | 17.68 | MTGL |
| ATOM | 492 | O   | ILE | 63 | 42.664 | -11.964 | 24.068 | 1.00 | 18.06 | MTGL |
| ATOM | 493 | N   | ALA | 64 | 43.722 | -12.058 | 26.046 | 1.00 | 17.70 | MTGL |
| ATOM | 494 | CA  | ALA | 64 | 43.379 | -13.463 | 26.253 | 1.00 | 17.86 | MTGL |
| ATOM | 495 | CB  | ALA | 64 | 44.000 | -13.971 | 27.555 | 1.00 | 17.49 | MTGL |
| ATOM | 496 | C   | ALA | 64 | 41.860 | -13.703 | 26.262 | 1.00 | 17.48 | MTGL |
| ATOM | 497 | O   | ALA | 64 | 41.370 | -14.616 | 25.599 | 1.00 | 17.31 | MTGL |
| ATOM | 498 | N   | ILE | 65 | 41.104 | -12.895 | 27.002 | 1.00 | 16.55 | MTGL |
| ATOM | 499 | CA  | ILE | 65 | 39.665 | -13.117 | 27.030 | 1.00 | 16.75 | MTGL |
| ATOM | 500 | CB  | ILE | 65 | 38.991 | -12.503 | 28.289 | 1.00 | 16.00 | MTGL |
| ATOM | 501 | CG2 | ILE | 65 | 39.574 | -13.130 | 29.536 | 1.00 | 16.34 | MTGL |
| ATOM | 502 | CG1 | ILE | 65 | 39.173 | -10.984 | 28.322 | 1.00 | 18.05 | MTGL |
| ATOM | 503 | CD1 | ILE | 65 | 38.423 | -10.321 | 29.474 | 1.00 | 15.44 | MTGL |
| ATOM | 504 | C   | ILE | 65 | 38.989 | -12.598 | 25.760 | 1.00 | 16.71 | MTGL |
| ATOM | 505 | O   | ILE | 65 | 37.938 | -13.101 | 25.368 | 1.00 | 16.21 | MTGL |
| ATOM | 506 | N   | ALA | 66 | 39.598 | -11.609 | 25.107 | 1.00 | 16.15 | MTGL |
| ATOM | 507 | CA  | ALA | 66 | 39.036 | -11.087 | 23.866 | 1.00 | 16.93 | MTGL |
| ATOM | 508 | CB  | ALA | 66 | 39.806 | -9.854  | 23.404 | 1.00 | 15.85 | MTGL |
| ATOM | 509 | C   | ALA | 66 | 39.106 | -12.185 | 22.802 | 1.00 | 17.72 | MTGL |
| ATOM | 510 | O   | ALA | 66 | 38.189 | -12.330 | 21.989 | 1.00 | 16.94 | MTGL |
| ATOM | 511 | N   | LYS | 67 | 40.188 | -12.965 | 22.817 | 1.00 | 18.09 | MTGL |
| ATOM | 512 | CA  | LYS | 67 | 40.340 | -14.059 | 21.856 | 1.00 | 19.65 | MTGL |
| ATOM | 513 | CB  | LYS | 67 | 41.700 | -14.748 | 22.010 | 1.00 | 21.06 | MTGL |
| ATOM | 514 | CG  | LYS | 67 | 42.892 | -13.953 | 21.484 | 1.00 | 23.60 | MTGL |
| ATOM | 515 | CD  | LYS | 67 | 44.159 | -14.795 | 21.550 | 1.00 | 26.88 | MTGL |
| ATOM | 516 | CE  | LYS | 67 | 45.365 | -14.050 | 21.000 | 1.00 | 29.59 | MTGL |
| ATOM | 517 | NZ  | LYS | 67 | 45.208 | -13.714 | 19.551 | 1.00 | 32.62 | MTGL |
| ATOM | 518 | C   | LYS | 67 | 39.229 | -15.085 | 22.070 | 1.00 | 19.44 | MTGL |
| ATOM | 519 | O   | LYS | 67 | 38.667 | -15.616 | 21.109 | 1.00 | 19.17 | MTGL |
| ATOM | 520 | N   | ARG | 68 | 38.921 | -15.365 | 23.335 | 1.00 | 18.94 | MTGL |
| ATOM | 521 | CA  | ARG | 68 | 37.866 | -16.317 | 23.672 | 1.00 | 17.61 | MTGL |

## Fig. 1 cont.

| ATOM | 522 | CB  | ARG | 68  | 37.834 | -16.567 | 25.181 | 1.00 | 16.99 | MTGL |
| ATOM | 523 | CG  | ARG | 68  | 38.950 | -17.488 | 25.679 | 1.00 | 18.79 | MTGL |
| ATOM | 524 | CD  | ARG | 68  | 39.015 | -17.515 | 27.199 | 1.00 | 17.89 | MTGL |
| ATOM | 525 | NE  | ARG | 68  | 37.742 | -17.892 | 27.809 | 1.00 | 18.08 | MTGL |
| ATOM | 526 | CZ  | ARG | 68  | 37.555 | -18.020 | 29.120 | 1.00 | 18.59 | MTGL |
| ATOM | 527 | NH1 | ARG | 68  | 38.561 | -17.798 | 29.961 | 1.00 | 18.68 | MTGL |
| ATOM | 528 | NH2 | ARG | 68  | 36.371 | -18.381 | 29.595 | 1.00 | 16.96 | MTGL |
| ATOM | 529 | C   | ARG | 68  | 36.511 | -15.799 | 23.209 | 1.00 | 17.25 | MTGL |
| ATOM | 530 | O   | ARG | 68  | 35.679 | -16.563 | 22.711 | 1.00 | 15.99 | MTGL |
| ATOM | 531 | N   | ALA | 69  | 36.285 | -14.503 | 23.395 | 1.00 | 16.95 | MTGL |
| ATOM | 532 | CA  | ALA | 69  | 35.030 | -13.886 | 22.982 | 1.00 | 18.21 | MTGL |
| ATOM | 533 | CB  | ALA | 69  | 35.001 | -12.411 | 23.393 | 1.00 | 18.02 | MTGL |
| ATOM | 534 | C   | ALA | 69  | 34.907 | -14.012 | 21.465 | 1.00 | 18.17 | MTGL |
| ATOM | 535 | O   | ALA | 69  | 33.867 | -14.407 | 20.945 | 1.00 | 16.83 | MTGL |
| ATOM | 536 | N   | LYS | 70  | 35.984 | -13.675 | 20.764 | 1.00 | 18.35 | MTGL |
| ATOM | 537 | CA  | LYS | 70  | 36.011 | -13.764 | 19.312 | 1.00 | 19.84 | MTGL |
| ATOM | 538 | CB  | LYS | 70  | 37.402 | -13.390 | 18.795 | 1.00 | 19.40 | MTGL |
| ATOM | 539 | CG  | LYS | 70  | 37.548 | -13.420 | 17.284 | 1.00 | 21.56 | MTGL |
| ATOM | 540 | CD  | LYS | 70  | 38.992 | -13.123 | 16.892 | 1.00 | 22.53 | MTGL |
| ATOM | 541 | CE  | LYS | 70  | 39.180 | -13.123 | 15.383 | 1.00 | 23.66 | MTGL |
| ATOM | 542 | NZ  | LYS | 70  | 40.592 | -12.852 | 15.015 | 1.00 | 21.95 | MTGL |
| ATOM | 543 | C   | LYS | 70  | 35.648 | -15.186 | 18.861 | 1.00 | 20.29 | MTGL |
| ATOM | 544 | O   | LYS | 70  | 34.842 | -15.365 | 17.948 | 1.00 | 19.93 | MTGL |
| ATOM | 545 | N   | ALA | 71  | 36.235 | -16.190 | 19.511 | 1.00 | 19.37 | MTGL |
| ATOM | 546 | CA  | ALA | 71· | 35.970 | -17.585 | 19.159 | 1.00 | 20.95 | MTGL |
| ATOM | 547 | CB  | ALA | 71  | 36.896 | -18.514 | 19.941 | 1.00 | 20.90 | MTGL |
| ATOM | 548 | C   | ALA | 71  | 34.514 | -17.975 | 19.405 | 1.00 | 21.38 | MTGL |
| ATOM | 549 | O   | ALA | 71  | 34.010 | -18.929 | 18.810 | 1.00 | 22.34 | MTGL |
| ATOM | 550 | N   | ALA | 72  | 33.839 | -17.244 | 20.282 | 1.00 | 20.63 | MTGL |
| ATOM | 551 | CA  | ALA | 72  | 32.439 | -17.529 | 20.574 | 1.00 | 20.92 | MTGL |
| ATOM | 552 | CB  | ALA | 72  | 32.149 | -17.284 | 22.050 | 1.00 | 20.20 | MTGL |
| ATOM | 553 | C   | ALA | 72  | 31.523 | -16.659 | 19.710 | 1.00 | 20.68 | MTGL |
| ATOM | 554 | O   | ALA | 72  | 30.305 | -16.644 | 19.899 | 1.00 | 20.23 | MTGL |
| ATOM | 555 | N   | GLY | 73  | 32.116 | -15.934 | 18.768 | 1.00 | 20.42 | MTGL |
| ATOM | 556 | CA  | GLY | 73  | 31.339 | -15.077 | 17.889 | 1.00 | 20.87 | MTGL |
| ATOM | 557 | C   | GLY | 73  | 30.874 | -13.774 | 18.523 | 1.00 | 21.42 | MTGL |
| ATOM | 558 | O   | GLY· | 73 | 29.946 | -13.133 | 18.027 | 1.00 | 21.96 | MTGL |
| ATOM | 559 | N   | LEU | 74  | 31.522 | -13.373 | 19.612 | 1.00 | 20.70 | MTGL |
| ATOM | 560 | CA  | LEU | 74  | 31.160 | -12.146 | 20.315 | 1.00 | 19.98 | MTGL |
| ATOM | 561 | CB  | LEU | 74  | 31.221 | -12.372 | 21.830 | 1.00 | 19.61 | MTGL |
| ATOM | 562 | CG  | LEU | 74  | 30.359 | -13.491 | 22.420 | 1.00 | 19.97 | MTGL |
| ATOM | 563 | CD1 | LEU | 74  | 30.692 | -13.659 | 23.898 | 1.00 | 19.32 | MTGL |
| ATOM | 564 | CD2 | LEU | 74  | 28.881 | -13.162 | 22.232 | 1.00 | 18.79 | MTGL |
| ATOM | 565 | C   | LEU | 74  | 32.071 | -10.978 | 19.960 | 1.00 | 19.91 | MTGL |
| ATOM | 566 | O   | LEU | 74  | 33.292 | -11.133 | 19.882 | 1.00 | 20.26 | MTGL |
| ATOM | 567 | N   | GLY | 75  | 31.473 | -9.809  | 19.740 | 1.00 | 19.06 | MTGL |
| ATOM | 568 | CA  | GLY | 75  | 32.261 | -8.627  | 19.438 | 1.00 | 18.36 | MTGL |
| ATOM | 569 | C   | GLY | 75  | 32.856 | -8.106  | 20.738 | 1.00 | 17.17 | MTGL |
| ATOM | 570 | O   | GLY | 75  | 32.380 | -8.457  | 21.821 | 1.00 | 16.83 | MTGL |
| ATOM | 571 | N   | VAL | 76  | 33.885 | -7.271  | 20.648 | 1.00 | 16.99 | MTGL |
| ATOM | 572 | CA  | VAL | 76  | 34.522 | -6.748  | 21.853 | 1.00 | 17.15 | MTGL |
| ATOM | 573 | CB  | VAL | 76  | 35.996 | -7.202  | 21.947 | 1.00 | 18.28 | MTGL |
| ATOM | 574 | CG1 | VAL | 76  | 36.626 | -6.682  | 23.238 | 1.00 | 17.92 | MTGL |
| ATOM | 575 | CG2 | VAL | 76  | 36.074 | -8.726  | 21.896 | 1.00 | 17.32 | MTGL |
| ATOM | 576 | C   | VAL | 76  | 34.476 | -5.231  | 21.984 | 1.00 | 17.67 | MTGL |
| ATOM | 577 | O   | VAL | 76  | 34.770 | -4.491  | 21.039 | 1.00 | 18.33 | MTGL |
| ATOM | 578 | N   | TYR | 77  | 34.108 | -4.785  | 23.177 | 1.00 | 16.77 | MTGL |
| ATOM | 579 | CA  | TYR | 77  | 34.013 | -3.366  | 23.517 | 1.00 | 16.63 | MTGL |

Fig. 1 cont.

| ATOM | 580 | CB | TYR | 77 | 32.608 | -3.102 | 24.097 | 1.00 | 15.27 | MTGL |
| ATOM | 581 | CG | TYR | 77 | 32.335 | -1.799 | 24.840 | 1.00 | 15.55 | MTGL |
| ATOM | 582 | CD1 | TYR | 77 | 33.343 | -0.886 | 25.149 | 1.00 | 15.39 | MTGL |
| ATOM | 583 | CE1 | TYR | 77 | 33.068 | 0.257 | 25.925 | 1.00 | 16.48 | MTGL |
| ATOM | 584 | CD2 | TYR | 77 | 31.046 | -1.532 | 25.312 | 1.00 | 16.02 | MTGL |
| ATOM | 585 | CE2 | TYR | 77 | 30.766 | -0.414 | 26.075 | 1.00 | 15.87 | MTGL |
| ATOM | 586 | CZ | TYR | 77 | 31.772 | 0.475 | 26.386 | 1.00 | 16.20 | MTGL |
| ATOM | 587 | OH | TYR | 77 | 31.471 | 1.541 | 27.200 | 1.00 | 15.93 | MTGL |
| ATOM | 588 | C | TYR | 77 | 35.114 | -3.128 | 24.548 | 1.00 | 16.00 | MTGL |
| ATOM | 589 | O | TYR | 77 | 35.026 | -3.604 | 25.683 | 1.00 | 16.53 | MTGL |
| ATOM | 590 | N | ILE | 78 | 36.163 | -2.419 | 24.142 | 1.00 | 16.29 | MTGL |
| ATOM | 591 | CA | ILE | 78 | 37.280 | -2.121 | 25.044 | 1.00 | 17.09 | MTGL |
| ATOM | 592 | CB | ILE | 78 | 38.611 | -2.008 | 24.261 | 1.00 | 17.14 | MTGL |
| ATOM | 593 | CG2 | ILE | 78 | 39.695 | -1.387 | 25.140 | 1.00 | 16.04 | MTGL |
| ATOM | 594 | CG1 | ILE | 78 | 39.049 | -3.394 | 23.777 | 1.00 | 16.84 | MTGL |
| ATOM | 595 | CD1 | ILE | 78 | 39.424 | -4.364 | 24.905 | 1.00 | 17.38 | MTGL |
| ATOM | 596 | C | ILE | 78 | 37.031 | -0.818 | 25.818 | 1.00 | 17.27 | MTGL |
| ATOM | 597 | O | ILE | 78 | 36.834 | 0.241 | 25.227 | 1.00 | 17.22 | MTGL |
| ATOM | 598 | N | ASP | 79 | 37.046 | -0.912 | 27.142 | 1.00 | 16.43 | MTGL |
| ATOM | 599 | CA | ASP | 79 | 36.817 | 0.234 | 28.009 | 1.00 | 16.05 | MTGL |
| ATOM | 600 | CB | ASP | 79 | 35.738 | -0.127 | 29.039 | 1.00 | 17.34 | MTGL |
| ATOM | 601 | CG | ASP | 79 | 35.577 | 0.920 | 30.133 | 1.00 | 19.18 | MTGL |
| ATOM | 602 | OD1 | ASP | 79 | 36.023 | 2.072 | 29.952 | 1.00 | 19.88 | MTGL |
| ATOM | 603 | OD2 | ASP | 79 | 34.986 | 0.583 | 31.181 | 1.00 | 20.19 | MTGL |
| ATOM | 604 | C | ASP | 79 | 38.113 | 0.657 | 28.699 | 1.00 | 16.01 | MTGL |
| ATOM | 605 | O | ASP | 79 | 38.479 | 0.102 | 29.732 | 1.00 | 15.54 | MTGL |
| ATOM | 606 | N | PHE | 80 | 38.810 | 1.626 | 28.105 | 1.00 | 15.57 | MTGL |
| ATOM | 607 | CA | PHE | 80 | 40.065 | 2.138 | 28.654 | 1.00 | 15.49 | MTGL |
| ATOM | 608 | CB | PHE | 80 | 40.811 | 3.005 | 27.627 | 1.00 | 14.72 | MTGL |
| ATOM | 609 | CG | PHE | 80 | 41.533 | 2.230 | 26.566 | 1.00 | 14.70 | MTGL |
| ATOM | 610 | CD1 | PHE | 80 | 42.548 | 1.343 | 26.899 | 1.00 | 14.82 | MTGL |
| ATOM | 611 | CD2 | PHE | 80 | 41.224 | 2.419 | 25.222 | 1.00 | 15.80 | MTGL |
| ATOM | 612 | CE1 | PHE | 80 | 43.251 | 0.649 | 25.912 | 1.00 | 15.54 | MTGL |
| ATOM | 613 | CE2 | PHE | 80 | 41.921 | 1.730 | 24.221 | 1.00 | 16.06 | MTGL |
| ATOM | 614 | CZ | PHE | 80 | 42.938 | 0.844 | 24.568 | 1.00 | 14.92 | MTGL |
| ATOM | 615 | C | PHE | 80 | 39.800 | 3.009 | 29.869 | 1.00 | 16.16 | MTGL |
| ATOM | 616 | O | PHE | 80 | 39.126 | 4.036 | 29.759 | 1.00 | 15.79 | MTGL |
| ATOM | 617 | N | HIS | 81 | 40.328 | 2.617 | 31.025 | 1.00 | 15.76 | MTGL |
| ATOM | 618 | CA | HIS | 81 | 40.140 | 3.419 | 32.234 | 1.00 | 15.04 | MTGL |
| ATOM | 619 | CB | HIS | 81 | 40.130 | 2.533 | 33.485 | 1.00 | 13.87 | MTGL |
| ATOM | 620 | CG | HIS | 81 | 38.846 | 1.790 | 33.686 | 1.00 | 14.70 | MTGL |
| ATOM | 621 | CD2 | HIS | 81 | 37.971 | 1.263 | 32.795 | 1.00 | 13.78 | MTGL |
| ATOM | 622 | ND1 | HIS | 81 | 38.312 | 1.554 | 34.933 | 1.00 | 13.45 | MTGL |
| ATOM | 623 | CE1 | HIS | 81 | 37.161 | 0.918 | 34.804 | 1.00 | 15.90 | MTGL |
| ATOM | 624 | NE2 | HIS | 81 | 36.931 | 0.730 | 33.516 | 1.00 | 14.78 | MTGL |
| ATOM | 625 | C | HIS | 81 | 41.244 | 4.466 | 32.357 | 1.00 | 15.46 | MTGL |
| ATOM | 626 | O | HIS | 81 | 41.113 | 5.439 | 33.102 | 1.00 | 14.94 | MTGL |
| ATOM | 627 | N | TYR | 82 | 42.326 | 4.273 | 31.609 | 1.00 | 15.09 | MTGL |
| ATOM | 628 | CA | TYR | 82 | 43.452 | 5.199 | 31.663 | 1.00 | 16.48 | MTGL |
| ATOM | 629 | CB | TYR | 82 | 43.092 | 6.520 | 30.974 | 1.00 | 15.74 | MTGL |
| ATOM | 630 | CG | TYR | 82 | 42.849 | 6.384 | 29.476 | 1.00 | 15.85 | MTGL |
| ATOM | 631 | CD1 | TYR | 82 | 43.702 | 5.615 | 28.680 | 1.00 | 15.30 | MTGL |
| ATOM | 632 | CE1 | TYR | 82 | 43.527 | 5.530 | 27.307 | 1.00 | 16.13 | MTGL |
| ATOM | 633 | CD2 | TYR | 82 | 41.801 | 7.062 | 28.852 | 1.00 | 15.60 | MTGL |
| ATOM | 634 | CE2 | TYR | 82 | 41.613 | 6.985 | 27.465 | 1.00 | 16.11 | MTGL |
| ATOM | 635 | CZ | TYR | 82 | 42.482 | 6.218 | 26.705 | 1.00 | 17.06 | MTGL |
| ATOM | 636 | OH | TYR | 82 | 42.331 | 6.148 | 25.345 | 1.00 | 18.86 | MTGL |
| ATOM | 637 | C | TYR | 82 | 43.866 | 5.437 | 33.122 | 1.00 | 17.11 | MTGL |

Fig. 1 cont.

| ATOM | 638 | O | TYR | 82 | 43.987 | 6.573 | 33.593 | 1.00 | 17.37 | MTGL |
|------|-----|-----|-----|-----|--------|--------|--------|------|-------|------|
| ATOM | 639 | N | SER | 83 | 44.077 | 4.329 | 33.822 | 1.00 | 17.17 | MTGL |
| ATOM | 640 | CA | SER | 83 | 44.482 | 4.328 | 35.223 | 1.00 | 17.21 | MTGL |
| ATOM | 641 | CB | SER | 83 | 43.288 | 4.679 | 36.115 | 1.00 | 16.41 | MTGL |
| ATOM | 642 | OG | SER | 83 | 43.639 | 4.651 | 37.487 | 1.00 | 16.64 | MTGL |
| ATOM | 643 | C | SER | 83 | 44.948 | 2.904 | 35.518 | 1.00 | 17.88 | MTGL |
| ATOM | 644 | O | SER | 83 | 44.689 | 1.993 | 34.732 | 1.00 | 17.59 | MTGL |
| ATOM | 645 | N | ASP | 84 | 45.646 | 2.706 | 36.630 | 1.00 | 18.00 | MTGL |
| ATOM | 646 | CA | ASP | 84 | 46.106 | 1.369 | 36.984 | 1.00 | 17.91 | MTGL |
| ATOM | 647 | CB | ASP | 84 | 47.378 | 1.415 | 37.840 | 1.00 | 18.31 | MTGL |
| ATOM | 648 | CG | ASP | 84 | 48.570 | 1.993 | 37.105 | 1.00 | 19.40 | MTGL |
| ATOM | 649 | OD1 | ASP | 84 | 48.732 | 1.724 | 35.897 | 1.00 | 18.50 | MTGL |
| ATOM | 650 | OD2 | ASP | 84 | 49.366 | 2.705 | 37.750 | 1.00 | 20.89 | MTGL |
| ATOM | 651 | C | ASP | 84 | 45.017 | 0.665 | 37.785 | 1.00 | 17.16 | MTGL |
| ATOM | 652 | O | ASP | 84 | 45.118 | -0.525 | 38.061 | 1.00 | 16.64 | MTGL |
| ATOM | 653 | N | THR | 85 | 43.978 | 1.406 | 38.152 | 1.00 | 16.98 | MTGL |
| ATOM | 654 | CA | THR | 85 | 42.889 | 0.837 | 38.943 | 1.00 | 17.09 | MTGL |
| ATOM | 655 | CB | THR | 85 | 43.169 | 1.056 | 40.456 | 1.00 | 17.53 | MTGL |
| ATOM | 656 | OG1 | THR | 85 | 42.211 | 0.337 | 41.239 | 1.00 | 20.04 | MTGL |
| ATOM | 657 | CG2 | THR | 85 | 43.107 | 2.549 | 40.805 | 1.00 | 16.84 | MTGL |
| ATOM | 658 | C | THR | 85 | 41.543 | 1.460 | 38.546 | 1.00 | 16.53 | MTGL |
| ATOM | 659 | O | THR | 85 | 41.481 | 2.245 | 37.598 | 1.00 | 16.58 | MTGL |
| ATOM | 660 | N | TRP | 86 | 40.477 | 1.100 | 39.264 | 1.00 | 15.91 | MTGL |
| ATOM | 661 | CA | TRP | 86 | 39.130 | 1.597 | 38.982 | 1.00 | 16.71 | MTGL |
| ATOM | 662 | CB | TRP | 86 | 38.166 | 1.291 | 40.143 | 1.00 | 15.33 | MTGL |
| ATOM | 663 | CG | TRP | 86 | 38.079 | -0.151 | 40.525 | 1.00 | 17.03 | MTGL |
| ATOM | 664 | CD2 | TRP | 86 | 37.311 | -1.165 | 39.871 | 1.00 | 16.85 | MTGL |
| ATOM | 665 | CE2 | TRP | 86 | 37.548 | -2.378 | 40.560 | 1.00 | 17.49 | MTGL |
| ATOM | 666 | CE3 | TRP | 86 | 36.448 | -1.170 | 38.767 | 1.00 | 16.06 | MTGL |
| ATOM | 667 | CD1 | TRP | 86 | 38.731 | -0.768 | 41.555 | 1.00 | 16.85 | MTGL |
| ATOM | 668 | NE1 | TRP | 86 | 38.417 | -2.104 | 41.583 | 1.00 | 17.28 | MTGL |
| ATOM | 669 | CZ2 | TRP | 86 | 36.951 | -3.588 | 40.180 | 1.00 | 16.23 | MTGL |
| ATOM | 670 | CZ3 | TRP | 86 | 35.853 | -2.373 | 38.388 | 1.00 | 17.14 | MTGL |
| ATOM | 671 | CH2 | TRP | 86 | 36.110 | -3.566 | 39.095 | 1.00 | 17.46 | MTGL |
| ATOM | 672 | C | TRP | 86 | 39.044 | 3.093 | 38.703 | 1.00 | 16.71 | MTGL |
| ATOM | 673 | O | TRP | 86 | 39.500 | 3.911 | 39.500 | 1.00 | 16.21 | MTGL |
| ATOM | 674 | N | ALA | 87 | 38.440 | 3.443 | 37.574 | 1.00 | 16.31 | MTGL |
| ATOM | 675 | CA | ALA | 87 | 38.249 | 4.845 | 37.223 | 1.00 | 17.57 | MTGL |
| ATOM | 676 | CB | ALA | 87 | 38.760 | 5.124 | 35.809 | 1.00 | 16.32 | MTGL |
| ATOM | 677 | C | ALA | 87 | 36.753 | 5.119 | 37.297 | 1.00 | 18.11 | MTGL |
| ATOM | 678 | O | ALA | 87 | 35.965 | 4.409 | 36.677 | 1.00 | 18.07 | MTGL |
| ATOM | 679 | N | ASP | 88 | 36.368 | 6.125 | 38.077 | 1.00 | 18.47 | MTGL |
| ATOM | 680 | CA | ASP | 88 | 34.965 | 6.512 | 38.213 | 1.00 | 18.85 | MTGL |
| ATOM | 681 | CB | ASP | 88 | 34.287 | 5.730 | 39.354 | 1.00 | 18.63 | MTGL |
| ATOM | 682 | CG | ASP | 88 | 35.047 | 5.816 | 40.661 | 1.00 | 19.12 | MTGL |
| ATOM | 683 | OD1 | ASP | 88 | 35.352 | 6.940 | 41.109 | 1.00 | 18.34 | MTGL |
| ATOM | 684 | OD2 | ASP | 88 | 35.331 | 4.749 | 41.248 | 1.00 | 19.72 | MTGL |
| ATOM | 685 | C | ASP | 88 | 34.932 | 8.021 | 38.460 | 1.00 | 18.13 | MTGL |
| ATOM | 686 | O | ASP | 88 | 35.980 | 8.656 | 38.505 | 1.00 | 17.65 | MTGL |
| ATOM | 687 | N | PRO | 89 | 33.737 | 8.616 | 38.615 | 1.00 | 18.93 | MTGL |
| ATOM | 688 | CD | PRO | 89 | 32.382 | 8.046 | 38.501 | 1.00 | 19.94 | MTGL |
| ATOM | 689 | CA | PRO | 89 | 33.672 | 10.066 | 38.842 | 1.00 | 19.49 | MTGL |
| ATOM | 690 | CB | PRO | 89 | 32.174 | 10.327 | 39.000 | 1.00 | 19.80 | MTGL |
| ATOM | 691 | CG | PRO | 89 | 31.555 | 9.263 | 38.125 | 1.00 | 19.69 | MTGL |
| ATOM | 692 | C | PRO | 89 | 34.476 | 10.600 | 40.025 | 1.00 | 19.90 | MTGL |
| ATOM | 693 | O | PRO | 89 | 34.833 | 11.778 | 40.048 | 1.00 | 20.62 | MTGL |
| ATOM | 694 | N | ALA | 90 | 34.760 | 9.743 | 40.999 | 1.00 | 18.70 | MTGL |
| ATOM | 695 | CA | ALA | 90 | 35.519 | 10.164 | 42.175 | 1.00 | 19.35 | MTGL |

Fig. 1 cont.

| ATOM | 696 | CB  | ALA | 90 | 34.818 | 9.685  | 43.457 | 1.00 | 17.48 | MTGL |
|------|-----|-----|-----|----|--------|--------|--------|------|-------|------|
| ATOM | 697 | C   | ALA | 90 | 36.964 | 9.674  | 42.162 | 1.00 | 18.63 | MTGL |
| ATOM | 698 | O   | ALA | 90 | 37.730 | 9.988  | 43.071 | 1.00 | 19.58 | MTGL |
| ATOM | 699 | N   | HIS | 91 | 37.333 | 8.901  | 41.145 | 1.00 | 17.84 | MTGL |
| ATOM | 700 | CA  | HIS | 91 | 38.698 | 8.391  | 41.039 | 1.00 | 17.68 | MTGL |
| ATOM | 701 | CB  | HIS | 91 | 38.833 | 7.000  | 41.679 | 1.00 | 18.34 | MTGL |
| ATOM | 702 | CG  | HIS | 91 | 38.298 | 6.910  | 43.072 | 1.00 | 20.31 | MTGL |
| ATOM | 703 | CD2 | HIS | 91 | 38.927 | 6.936  | 44.272 | 1.00 | 19.87 | MTGL |
| ATOM | 704 | ND1 | HIS | 91 | 36.953 | 6.784  | 43.344 | 1.00 | 18.50 | MTGL |
| ATOM | 705 | CE1 | HIS | 91 | 36.775 | 6.736  | 44.653 | 1.00 | 20.43 | MTGL |
| ATOM | 706 | NE2 | HIS | 91 | 37.956 | 6.826  | 45.238 | 1.00 | 21.64 | MTGL |
| ATOM | 707 | C   | HIS | 91 | 39.177 | 8.280  | 39.597 | 1.00 | 16.55 | MTGL |
| ATOM | 708 | O   | HIS | 91 | 38.661 | 7.478  | 38.823 | 1.00 | 16.39 | MTGL |
| ATOM | 709 | N   | GLN | 92 | 40.169 | 9.087  | 39.246 | 1.00 | 15.52 | MTGL |
| ATOM | 710 | CA  | GLN | 92 | 40.760 | 9.064  | 37.911 | 1.00 | 15.68 | MTGL |
| ATOM | 711 | CB  | GLN | 92 | 40.281 | 10.255 | 37.072 | 1.00 | 14.49 | MTGL |
| ATOM | 712 | CG  | GLN | 92 | 38.786 | 10.229 | 36.702 | 1.00 | 13.93 | MTGL |
| ATOM | 713 | CD  | GLN | 92 | 38.413 | 9.127  | 35.699 | 1.00 | 14.84 | MTGL |
| ATOM | 714 | OE1 | GLN | 92 | 39.173 | 8.814  | 34.779 | 1.00 | 15.41 | MTGL |
| ATOM | 715 | NE2 | GLN | 92 | 37.221 | 8.559  | 35.861 | 1.00 | 14.23 | MTGL |
| ATOM | 716 | C   | GLN | 92 | 42.254 | 9.166  | 38.190 | 1.00 | 15.81 | MTGL |
| ATOM | 717 | O   | GLN | 92 | 42.925 | 10.108 | 37.782 | 1.00 | 16.26 | MTGL |
| ATOM | 718 | N   | THR | 93 | 42.759 | 8.169  | 38.902 | 1.00 | 16.47 | MTGL |
| ATOM | 719 | CA  | THR | 93 | 44.156 | 8.136  | 39.302 | 1.00 | 17.33 | MTGL |
| ATOM | 720 | CB  | THR | 93 | 44.387 | 7.062  | 40.364 | 1.00 | 17.41 | MTGL |
| ATOM | 721 | OG1 | THR | 93 | 43.433 | 7.239  | 41.417 | 1.00 | 19.90 | MTGL |
| ATOM | 722 | CG2 | THR | 93 | 45.800 | 7.177  | 40.944 | 1.00 | 19.68 | MTGL |
| ATOM | 723 | C   | THR | 93 | 45.136 | 7.925  | 38.165 | 1.00 | 17.55 | MTGL |
| ATOM | 724 | O   | THR | 93 | 45.035 | 6.973  | 37.390 | 1.00 | 17.01 | MTGL |
| ATOM | 725 | N   | MET | 94 | 46.093 | 8.839  | 38.089 | 1.00 | 17.63 | MTGL |
| ATOM | 726 | CA  | MET | 94 | 47.131 | 8.820  | 37.079 | 1.00 | 18.68 | MTGL |
| ATOM | 727 | CB  | MET | 94 | 48.144 | 9.926  | 37.383 | 1.00 | 21.10 | MTGL |
| ATOM | 728 | CG  | MET | 94 | 49.195 | 10.133 | 36.315 | 1.00 | 23.55 | MTGL |
| ATOM | 729 | SD  | MET | 94 | 48.474 | 10.956 | 34.894 | 1.00 | 27.41 | MTGL |
| ATOM | 730 | CE  | MET | 94 | 48.342 | 12.657 | 35.533 | 1.00 | 25.13 | MTGL |
| ATOM | 731 | C   | MET | 94 | 47.854 | 7.476  | 37.064 | 1.00 | 18.43 | MTGL |
| ATOM | 732 | O   | MET | 94 | 48.179 | 6.925  | 38.113 | 1.00 | 18.13 | MTGL |
| ATOM | 733 | N   | PRO | 95 | 48.088 | 6.914  | 35.871 | 1.00 | 17.41 | MTGL |
| ATOM | 734 | CD  | PRO | 95 | 47.534 | 7.255  | 34.551 | 1.00 | 16.67 | MTGL |
| ATOM | 735 | CA  | PRO | 95 | 48.797 | 5.631  | 35.834 | 1.00 | 17.83 | MTGL |
| ATOM | 736 | CB  | PRO | 95 | 48.814 | 5.287  | 34.347 | 1.00 | 17.25 | MTGL |
| ATOM | 737 | CG  | PRO | 95 | 47.544 | 5.914  | 33.843 | 1.00 | 17.35 | MTGL |
| ATOM | 738 | C   | PRO | 95 | 50.202 | 5.903  | 36.371 | 1.00 | 18.71 | MTGL |
| ATOM | 739 | O   | PRO | 95 | 50.784 | 6.952  | 36.084 | 1.00 | 17.30 | MTGL |
| ATOM | 740 | N   | ALA | 96 | 50.746 | 4.978  | 37.152 | 1.00 | 18.59 | MTGL |
| ATOM | 741 | CA  | ALA | 96 | 52.082 | 5.177  | 37.705 | 1.00 | 20.01 | MTGL |
| ATOM | 742 | CB  | ALA | 96 | 52.470 | 3.983  | 38.587 | 1.00 | 19.66 | MTGL |
| ATOM | 743 | C   | ALA | 96 | 53.095 | 5.357  | 36.577 | 1.00 | 20.37 | MTGL |
| ATOM | 744 | O   | ALA | 96 | 53.081 | 4.617  | 35.595 | 1.00 | 20.80 | MTGL |
| ATOM | 745 | N   | GLY | 97 | 53.959 | 6.356  | 36.710 | 1.00 | 20.53 | MTGL |
| ATOM | 746 | CA  | GLY | 97 | 54.967 | 6.595  | 35.693 | 1.00 | 20.43 | MTGL |
| ATOM | 747 | C   | GLY | 97 | 54.611 | 7.644  | 34.654 | 1.00 | 20.83 | MTGL |
| ATOM | 748 | O   | GLY | 97 | 55.491 | 8.144  | 33.959 | 1.00 | 22.30 | MTGL |
| ATOM | 749 | N   | TRP | 98 | 53.332 | 7.982  | 34.537 | 1.00 | 20.23 | MTGL |
| ATOM | 750 | CA  | TRP | 98 | 52.902 | 8.978  | 33.561 | 1.00 | 19.86 | MTGL |
| ATOM | 751 | CB  | TRP | 98 | 51.415 | 8.795  | 33.249 | 1.00 | 18.17 | MTGL |
| ATOM | 752 | CG  | TRP | 98 | 51.106 | 7.576  | 32.421 | 1.00 | 17.34 | MTGL |
| ATOM | 753 | CD2 | TRP | 98 | 49.987 | 7.397  | 31.543 | 1.00 | 16.19 | MTGL |

Fig. 1 cont.

| ATOM | 754 | CE2 | TRP | 98 | 50.082 | 6.093 | 31.006 | 1.00 | 16.95 | MTGL |
|------|-----|-----|-----|-----|--------|-------|--------|------|-------|------|
| ATOM | 755 | CE3 | TRP | 98 | 48.914 | 8.213 | 31.156 | 1.00 | 15.48 | MTGL |
| ATOM | 756 | CD1 | TRP | 98 | 51.810 | 6.406 | 32.385 | 1.00 | 18.21 | MTGL |
| ATOM | 757 | NE1 | TRP | 98 | 51.202 | 5.511 | 31.538 | 1.00 | 17.45 | MTGL |
| ATOM | 758 | CZ2 | TRP | 98 | 49.140 | 5.580 | 30.103 | 1.00 | 17.12 | MTGL |
| ATOM | 759 | CZ3 | TRP | 98 | 47.974 | 7.704 | 30.257 | 1.00 | 15.71 | MTGL |
| ATOM | 760 | CH2 | TRP | 98 | 48.098 | 6.399 | 29.740 | 1.00 | 16.54 | MTGL |
| ATOM | 761 | C | TRP | 98 | 53.156 | 10.401 | 34.056 | 1.00 | 20.28 | MTGL |
| ATOM | 762 | O | TRP | 98 | 52.958 | 10.706 | 35.230 | 1.00 | 19.92 | MTGL |
| ATOM | 763 | N | PRO | 99 | 53.593 | 11.295 | 33.156 | 1.00 | 21.71 | MTGL |
| ATOM | 764 | CD | PRO | 99 | 53.852 | 11.048 | 31.725 | 1.00 | 22.15 | MTGL |
| ATOM | 765 | CA | PRO | 99 | 53.875 | 12.693 | 33.505 | 1.00 | 22.69 | MTGL |
| ATOM | 766 | CB | PRO | 99 | 54.610 | 13.205 | 32.269 | 1.00 | 22.58 | MTGL |
| ATOM | 767 | CG | PRO | 99 | 53.938 | 12.454 | 31.163 | 1.00 | 22.80 | MTGL |
| ATOM | 768 | C | PRO | 99 | 52.598 | 13.483 | 33.797 | 1.00 | 23.10 | MTGL |
| ATOM | 769 | O | PRO | 99 | 51.530 | 13.156 | 33.277 | 1.00 | 23.44 | MTGL |
| ATOM | 770 | N | SER | 100 | 52.716 | 14.522 | 34.621 | 1.00 | 22.96 | MTGL |
| ATOM | 771 | CA | SER | 100 | 51.572 | 15.353 | 34.995 | 1.00 | 23.06 | MTGL |
| ATOM | 772 | CB | SER | 100 | 51.714 | 15.831 | 36.445 | 1.00 | 24.32 | MTGL |
| ATOM | 773 | OG | SER | 100 | 51.658 | 14.746 | 37.353 | 1.00 | 26.38 | MTGL |
| ATOM | 774 | C | SER | 100 | 51.332 | 16.574 | 34.115 | 1.00 | 22.44 | MTGL |
| ATOM | 775 | O | SER | 100 | 50.202 | 17.051 | 34.032 | 1.00 | 22.25 | MTGL |
| ATOM | 776 | N | ASP | 101 | 52.379 | 17.098 | 33.480 | 1.00 | 22.38 | MTGL |
| ATOM | 777 | CA | ASP | 101 | 52.208 | 18.283 | 32.639 | 1.00 | 23.28 | MTGL |
| ATOM | 778 | CB | ASP | 101 | 53.565 | 18.890 | 32.254 | 1.00 | 24.51 | MTGL |
| ATOM | 779 | CG | ASP | 101 | 54.382 | 17.986 | 31.352 | 1.00 | 25.84 | MTGL |
| ATOM | 780 | OD1 | ASP | 101 | 54.886 | 16.954 | 31.842 | 1.00 | 26.46 | MTGL |
| ATOM | 781 | OD2 | ASP | 101 | 54.515 | 18.310 | 30.152 | 1.00 | 25.84 | MTGL |
| ATOM | 782 | C | ASP | 101 | 51.411 | 17.933 | 31.386 | 1.00 | 22.28 | MTGL |
| ATOM | 783 | O | ASP | 101 | 51.667 | 16.915 | 30.743 | 1.00 | 21.59 | MTGL |
| ATOM | 784 | N | ILE | 102 | 50.452 | 18.787 | 31.042 | 1.00 | 21.77 | MTGL |
| ATOM | 785 | CA | ILE | 102 | 49.584 | 18.548 | 29.890 | 1.00 | 21.42 | MTGL |
| ATOM | 786 | CB | ILE | 102 | 48.623 | 19.738 | 29.663 | 1.00 | 20.48 | MTGL |
| ATOM | 787 | CG2 | ILE | 102 | 49.411 | 20.998 | 29.313 | 1.00 | 20.99 | MTGL |
| ATOM | 788 | CG1 | ILE | 102 | 47.617 | 19.392 | 28.560 | 1.00 | 21.44 | MTGL |
| ATOM | 789 | CD1 | ILE | 102 | 46.730 | 18.200 | 28.879 | 1.00 | 19.62 | MTGL |
| ATOM | 790 | C | ILE | 102 | 50.281 | 18.196 | 28.573 | 1.00 | 21.71 | MTGL |
| ATOM | 791 | O | ILE | 102 | 49.861 | 17.258 | 27.896 | 1.00 | 20.84 | MTGL |
| ATOM | 792 | N | ASP | 103 | 51.336 | 18.918 | 28.201 | 1.00 | 21.01 | MTGL |
| ATOM | 793 | CA | ASP | 103 | 52.012 | 18.608 | 26.945 | 1.00 | 22.44 | MTGL |
| ATOM | 794 | CB | ASP | 103 | 53.219 | 19.523 | 26.716 | 1.00 | 24.91 | MTGL |
| ATOM | 795 | CG | ASP | 103 | 52.821 | 20.942 | 26.370 | 1.00 | 27.06 | MTGL |
| ATOM | 796 | OD1 | ASP | 103 | 51.633 | 21.178 | 26.070 | 1.00 | 27.99 | MTGL |
| ATOM | 797 | OD2 | ASP | 103 | 53.703 | 21.823 | 26.385 | 1.00 | 28.69 | MTGL |
| ATOM | 798 | C | ASP | 103 | 52.478 | 17.160 | 26.886 | 1.00 | 22.61 | MTGL |
| ATOM | 799 | O | ASP | 103 | 52.144 | 16.435 | 25.948 | 1.00 | 23.39 | MTGL |
| ATOM | 800 | N | ASN | 104 | 53.244 | 16.734 | 27.885 | 1.00 | 21.79 | MTGL |
| ATOM | 801 | CA | ASN | 104 | 53.751 | 15.366 | 27.898 | 1.00 | 22.22 | MTGL |
| ATOM | 802 | CB | ASN | 104 | 54.912 | 15.244 | 28.884 | 1.00 | 23.92 | MTGL |
| ATOM | 803 | CG | ASN | 104 | 56.149 | 15.977 | 28.406 | 1.00 | 26.18 | MTGL |
| ATOM | 804 | OD1 | ASN | 104 | 56.715 | 15.643 | 27.364 | 1.00 | 26.60 | MTGL |
| ATOM | 805 | ND2 | ASN | 104 | 56.570 | 16.989 | 29.157 | 1.00 | 26.07 | MTGL |
| ATOM | 806 | C | ASN | 104 | 52.699 | 14.311 | 28.191 | 1.00 | 21.08 | MTGL |
| ATOM | 807 | O | ASN | 104 | 52.774 | 13.210 | 27.655 | 1.00 | 20.89 | MTGL |
| ATOM | 808 | N | LEU | 105 | 51.722 | 14.642 | 29.032 | 1.00 | 20.18 | MTGL |
| ATOM | 809 | CA | LEU | 105 | 50.663 | 13.693 | 29.361 | 1.00 | 19.91 | MTGL |
| ATOM | 810 | CB | LEU | 105 | 49.743 | 14.249 | 30.452 | 1.00 | 17.16 | MTGL |
| ATOM | 811 | CG | LEU | 105 | 48.568 | 13.339 | 30.842 | 1.00 | 18.64 | MTGL |

## Fig. 1 cont.

| ATOM | 812 | CD1 | LEU | 105 | 49.089 | 12.019 | 31.413 | 1.00 | 15.72 | MTGL |
|------|-----|-----|-----|-----|--------|--------|--------|------|-------|------|
| ATOM | 813 | CD2 | LEU | 105 | 47.690 | 14.040 | 31.860 | 1.00 | 17.06 | MTGL |
| ATOM | 814 | C | LEU | 105 | 49.841 | 13.392 | 28.109 | 1.00 | 20.55 | MTGL |
| ATOM | 815 | O | LEU | 105 | 49.506 | 12.237 | 27.839 | 1.00 | 20.48 | MTGL |
| ATOM | 816 | N | SER | 106 | 49.521 | 14.435 | 27.346 | 1.00 | 20.24 | MTGL |
| ATOM | 817 | CA | SER | 106 | 48.746 | 14.264 | 26.124 | 1.00 | 21.47 | MTGL |
| ATOM | 818 | CB | SER | 106 | 48.514 | 15.610 | 25.437 | 1.00 | 22.23 | MTGL |
| ATOM | 819 | OG | SER | 106 | 47.695 | 16.447 | 26.235 | 1.00 | 27.30 | MTGL |
| ATOM | 820 | C | SER | 106 | 49.484 | 13.338 | 25.173 | 1.00 | 20.88 | MTGL |
| ATOM | 821 | O | SER | 106 | 48.884 | 12.487 | 24.527 | 1.00 | 19.42 | MTGL |
| ATOM | 822 | N | TRP | 107 | 50.795 | 13.513 | 25.096 | 1.00 | 22.85 | MTGL |
| ATOM | 823 | CA | TRP | 107 | 51.623 | 12.696 | 24.223 | 1.00 | 24.06 | MTGL |
| ATOM | 824 | CB | TRP | 107 | 53.033 | 13.282 | 24.164 | 1.00 | 27.94 | MTGL |
| ATOM | 825 | CG | TRP | 107 | 53.780 | 12.934 | 22.924 | 1.00 | 32.46 | MTGL |
| ATOM | 826 | CD2 | TRP | 107 | 55.136 | 13.276 | 22.621 | 1.00 | 35.03 | MTGL |
| ATOM | 827 | CE2 | TRP | 107 | 55.414 | 12.776 | 21.328 | 1.00 | 36.06 | MTGL |
| ATOM | 828 | CE3 | TRP | 107 | 56.141 | 13.971 | 23.309 | 1.00 | 36.31 | MTGL |
| ATOM | 829 | CD1 | TRP | 107 | 53.303 | 12.249 | 21.839 | 1.00 | 33.32 | MTGL |
| ATOM | 830 | NE1 | TRP | 107 | 54.280 | 12.148 | 20.877 | 1.00 | 35.87 | MTGL |
| ATOM | 831 | CZ2 | TRP | 107 | 56.662 | 12.934 | 20.715 | 1.00 | 36.87 | MTGL |
| ATOM | 832 | CZ3 | TRP | 107 | 57.381 | 14.130 | 22.698 | 1.00 | 37.64 | MTGL |
| ATOM | 833 | CH2 | TRP | 107 | 57.627 | 13.617 | 21.410 | 1.00 | 37.50 | MTGL |
| ATOM | 834 | C | TRP | 107 | 51.674 | 11.250 | 24.725 | 1.00 | 23.66 | MTGL |
| ATOM | 835 | O | TRP | 107 | 51.632 | 10.306 | 23.929 | 1.00 | 22.42 | MTGL |
| ATOM | 836 | N | LYS | 108 | 51.754 | 11.085 | 26.045 | 1.00 | 21.87 | MTGL |
| ATOM | 837 | CA | LYS | 108 | 51.810 | 9.758 | 26.654 | 1.00 | 21.77 | MTGL |
| ATOM | 838 | CB | LYS | 108 | 52.012 | 9.870 | 28.167 | 1.00 | 22.68 | MTGL |
| ATOM | 839 | CG | LYS | 108 | 52.928 | 8.818 | 28.787 | 1.00 | 25.44 | MTGL |
| ATOM | 840 | CD | LYS | 108 | 52.756 | 7.420 | 28.208 | 1.00 | 25.37 | MTGL |
| ATOM | 841 | CE | LYS | 108 | 53.657 | 6.436 | 28.948 | 1.00 | 26.82 | MTGL |
| ATOM | 842 | NZ | LYS | 108 | 53.912 | 5.168 | 28.202 | 1.00 | 25.16 | MTGL |
| ATOM | 843 | C | LYS | 108 | 50.502 | 9.016 | 26.400 | 1.00 | 21.11 | MTGL |
| ATOM | 844 | O | LYS | 108 | 50.499 | 7.825 | 26.082 | 1.00 | 20.02 | MTGL |
| ATOM | 845 | N | LEU | 109 | 49.394 | 9.733 | 26.569 | 1.00 | 20.01 | MTGL |
| ATOM | 846 | CA | LEU | 109 | 48.069 | 9.165 | 26.378 | 1.00 | 19.28 | MTGL |
| ATOM | 847 | CB | LEU | 109 | 46.998 | 10.210 | 26.701 | 1.00 | 17.83 | MTGL |
| ATOM | 848 | CG | LEU | 109 | 45.541 | 9.782 | 26.544 | 1.00 | 18.16 | MTGL |
| ATOM | 849 | CD1 | LEU | 109 | 45.278 | 8.500 | 27.331 | 1.00 | 16.64 | MTGL |
| ATOM | 850 | CD2 | LEU | 109 | 44.639 | 10.912 | 27.023 | 1.00 | 17.12 | MTGL |
| ATOM | 851 | C | LEU | 109 | 47.922 | 8.689 | 24.941 | 1.00 | 19.15 | MTGL |
| ATOM | 852 | O | LEU | 109 | 47.356 | 7.630 | 24.681 | 1.00 | 17.95 | MTGL |
| ATOM | 853 | N | TYR | 110 | 48.439 | 9.485 | 24.013 | 1.00 | 19.31 | MTGL |
| ATOM | 854 | CA | TYR | 110 | 48.390 | 9.141 | 22.602 | 1.00 | 20.23 | MTGL |
| ATOM | 855 | CB | TYR | 110 | 48.928 | 10.308 | 21.765 | 1.00 | 20.77 | MTGL |
| ATOM | 856 | CG | TYR | 110 | 49.112 | 9.988 | 20.301 | 1.00 | 22.28 | MTGL |
| ATOM | 857 | CD1 | TYR | 110 | 50.324 | 9.483 | 19.827 | 1.00 | 22.42 | MTGL |
| ATOM | 858 | CE1 | TYR | 110 | 50.500 | 9.174 | 18.478 | 1.00 | 23.01 | MTGL |
| ATOM | 859 | CD2 | TYR | 110 | 48.072 | 10.179 | 19.388 | 1.00 | 21.90 | MTGL |
| ATOM | 860 | CE2 | TYR | 110 | 48.236 | 9.873 | 18.033 | 1.00 | 22.98 | MTGL |
| ATOM | 861 | CZ | TYR | 110 | 49.453 | 9.373 | 17.589 | 1.00 | 22.70 | MTGL |
| ATOM | 862 | OH | TYR | 110 | 49.628 | 9.075 | 16.261 | 1.00 | 22.60 | MTGL |
| ATOM | 863 | C | TYR | 110 | 49.209 | 7.873 | 22.351 | 1.00 | 20.36 | MTGL |
| ATOM | 864 | O | TYR | 110 | 48.713 | 6.915 | 21.753 | 1.00 | 19.75 | MTGL |
| ATOM | 865 | N | ASN | 111 | 50.453 | 7.864 | 22.826 | 1.00 | 19.95 | MTGL |
| ATOM | 866 | CA | ASN | 111 | 51.333 | 6.712 | 22.650 | 1.00 | 20.79 | MTGL |
| ATOM | 867 | CB | ASN | 111 | 52.691 | 6.944 | 23.316 | 1.00 | 22.26 | MTGL |
| ATOM | 868 | CG | ASN | 111 | 53.496 | 8.030 | 22.642 | 1.00 | 26.38 | MTGL |
| ATOM | 869 | OD1 | ASN | 111 | 53.175 | 8.463 | 21.534 | 1.00 | 25.33 | MTGL |

# Fig. 1 cont.

| ATOM | 870 | ND2 | ASN | 111 | 54.556 | 8.463 | 23.317 | 1.00 | 29.11 | MTGL |
|------|-----|-----|-----|-----|--------|-------|--------|------|-------|------|
| ATOM | 871 | C   | ASN | 111 | 50.736 | 5.445 | 23.234 | 1.00 | 20.44 | MTGL |
| ATOM | 872 | O   | ASN | 111 | 50.764 | 4.391 | 22.605 | 1.00 | 20.22 | MTGL |
| ATOM | 873 | N   | TYR | 112 | 50.218 | 5.551 | 24.452 | 1.00 | 19.27 | MTGL |
| ATOM | 874 | CA  | TYR | 112 | 49.622 | 4.406 | 25.123 | 1.00 | 18.94 | MTGL |
| ATOM | 875 | CB  | TYR | 112 | 49.131 | 4.801 | 26.517 | 1.00 | 16.74 | MTGL |
| ATOM | 876 | CG  | TYR | 112 | 48.211 | 3.770 | 27.137 | 1.00 | 17.22 | MTGL |
| ATOM | 877 | CD1 | TYR | 112 | 48.723 | 2.632 | 27.766 | 1.00 | 15.42 | MTGL |
| ATOM | 878 | CE1 | TYR | 112 | 47.876 | 1.671 | 28.311 | 1.00 | 17.32 | MTGL |
| ATOM | 879 | CD2 | TYR | 112 | 46.827 | 3.916 | 27.065 | 1.00 | 15.87 | MTGL |
| ATOM | 880 | CE2 | TYR | 112 | 45.971 | 2.960 | 27.604 | 1.00 | 17.72 | MTGL |
| ATOM | 881 | CZ  | TYR | 112 | 46.500 | 1.844 | 28.225 | 1.00 | 16.39 | MTGL |
| ATOM | 882 | OH  | TYR | 112 | 45.653 | 0.907 | 28.766 | 1.00 | 18.06 | MTGL |
| ATOM | 883 | C   | TYR | 112 | 48.449 | 3.832 | 24.330 | 1.00 | 18.50 | MTGL |
| ATOM | 884 | O   | TYR | 112 | 48.358 | 2.622 | 24.129 | 1.00 | 17.86 | MTGL |
| ATOM | 885 | N   | THR | 113 | 47.545 | 4.709 | 23.903 | 1.00 | 18.56 | MTGL |
| ATOM | 886 | CA  | THR | 113 | 46.372 | 4.288 | 23.152 | 1.00 | 18.24 | MTGL |
| ATOM | 887 | CB  | THR | 113 | 45.408 | 5.474 | 22.930 | 1.00 | 17.98 | MTGL |
| ATOM | 888 | OG1 | THR | 113 | 45.017 | 6.014 | 24.198 | 1.00 | 16.20 | MTGL |
| ATOM | 889 | CG2 | THR | 113 | 44.158 | 5.021 | 22.184 | 1.00 | 17.01 | MTGL |
| ATOM | 890 | C   | THR | 113 | 46.765 | 3.682 | 21.805 | 1.00 | 18.67 | MTGL |
| ATOM | 891 | O   | THR | 113 | 46.272 | 2.619 | 21.423 | 1.00 | 18.43 | MTGL |
| ATOM | 892 | N   | LEU | 114 | 47.655 | 4.360 | 21.090 | 1.00 | 19.14 | MTGL |
| ATOM | 893 | CA  | LEU | 114 | 48.114 | 3.873 | 19.797 | 1.00 | 20.50 | MTGL |
| ATOM | 894 | CB  | LEU | 114 | 49.133 | 4.848 | 19.197 | 1.00 | 20.12 | MTGL |
| ATOM | 895 | CG  | LEU | 114 | 49.864 | 4.396 | 17.929 | 1.00 | 21.74 | MTGL |
| ATOM | 896 | CD1 | LEU | 114 | 48.866 | 4.214 | 16.794 | 1.00 | 21.80 | MTGL |
| ATOM | 897 | CD2 | LEU | 114 | 50.924 | 5.430 | 17.547 | 1.00 | 22.25 | MTGL |
| ATOM | 898 | C   | LEU | 114 | 48.753 | 2.498 | 19.984 | 1.00 | 20.96 | MTGL |
| ATOM | 899 | O   | LEU | 114 | 48.441 | 1.551 | 19.263 | 1.00 | 21.53 | MTGL |
| ATOM | 900 | N   | ASP | 115 | 49.650 | 2.399 | 20.961 | 1.00 | 21.00 | MTGL |
| ATOM | 901 | CA  | ASP | 115 | 50.335 | 1.148 | 21.252 | 1.00 | 21.18 | MTGL |
| ATOM | 902 | CB  | ASP | 115 | 51.276 | 1.331 | 22.442 | 1.00 | 22.68 | MTGL |
| ATOM | 903 | CG  | ASP | 115 | 51.957 | 0.041 | 22.843 | 1.00 | 24.76 | MTGL |
| ATOM | 904 | OD1 | ASP | 115 | 52.826 | -0.429| 22.078 | 1.00 | 26.71 | MTGL |
| ATOM | 905 | OD2 | ASP | 115 | 51.616 | -0.509| 23.917 | 1.00 | 25.94 | MTGL |
| ATOM | 906 | C   | ASP | 115 | 49.351 | 0.018 | 21.561 | 1.00 | 21.01 | MTGL |
| ATOM | 907 | O   | ASP | 115 | 49.461 | -1.078| 21.012 | 1.00 | 20.38 | MTGL |
| ATOM | 908 | N   | ALA | 116 | 48.404 | 0.287 | 22.456 | 1.00 | 19.72 | MTGL |
| ATOM | 909 | CA  | ALA | 116 | 47.410 | -0.711| 22.833 | 1.00 | 19.79 | MTGL |
| ATOM | 910 | CB  | ALA | 116 | 46.501 | -0.163| 23.923 | 1.00 | 19.04 | MTGL |
| ATOM | 911 | C   | ALA | 116 | 46.578 | -1.140| 21.627 | 1.00 | 18.78 | MTGL |
| ATOM | 912 | O   | ALA | 116 | 46.302 | -2.323| 21.448 | 1.00 | 18.71 | MTGL |
| ATOM | 913 | N   | ALA | 117 | 46.184 | -0.172| 20.806 | 1.00 | 18.51 | MTGL |
| ATOM | 914 | CA  | ALA | 117 | 45.384 | -0.456| 19.616 | 1.00 | 19.07 | MTGL |
| ATOM | 915 | CB  | ALA | 117 | 45.012 | 0.840 | 18.913 | 1.00 | 17.76 | MTGL |
| ATOM | 916 | C   | ALA | 117 | 46.144 | -1.372| 18.662 | 1.00 | 19.00 | MTGL |
| ATOM | 917 | O   | ALA | 117 | 45.588 | -2.344| 18.157 | 1.00 | 20.94 | MTGL |
| ATOM | 918 | N   | ASN | 118 | 47.414 | -1.064| 18.421 | 1.00 | 19.11 | MTGL |
| ATOM | 919 | CA  | ASN | 118 | 48.234 | -1.880| 17.530 | 1.00 | 20.09 | MTGL |
| ATOM | 920 | CB  | ASN | 118 | 49.594 | -1.214| 17.280 | 1.00 | 19.53 | MTGL |
| ATOM | 921 | CG  | ASN | 118 | 49.481 | 0.043 | 16.432 | 1.00 | 21.06 | MTGL |
| ATOM | 922 | OD1 | ASN | 118 | 48.591 | 0.158 | 15.584 | 1.00 | 22.85 | MTGL |
| ATOM | 923 | ND2 | ASN | 118 | 50.394 | 0.984 | 16.644 | 1.00 | 19.62 | MTGL |
| ATOM | 924 | C   | ASN | 118 | 48.446 | -3.294| 18.069 | 1.00 | 20.53 | MTGL |
| ATOM | 925 | O   | ASN | 118 | 48.509 | -4.250| 17.298 | 1.00 | 20.72 | MTGL |
| ATOM | 926 | N   | LYS | 119 | 48.570 | -3.427| 19.389 | 1.00 | 20.26 | MTGL |
| ATOM | 927 | CA  | LYS | 119 | 48.755 | -4.745| 19.992 | 1.00 | 19.69 | MTGL |

Fig. 1 cont.

| ATOM | 928 | CB | LYS | 119 | 49.134 | -4.616 | 21.468 | 1.00 | 20.25 | MTGL |
|------|-----|-----|-----|-----|--------|--------|--------|------|-------|------|
| ATOM | 929 | CG | LYS | 119 | 50.589 | -4.225 | 21.668 | 1.00 | 23.15 | MTGL |
| ATOM | 930 | CD | LYS | 119 | 50.933 | -4.015 | 23.131 | 1.00 | 25.43 | MTGL |
| ATOM | 931 | CE | LYS | 119 | 52.378 | -3.533 | 23.273 | 1.00 | 26.95 | MTGL |
| ATOM | 932 | NZ | LYS | 119 | 52.701 | -3.126 | 24.666 | 1.00 | 26.48 | MTGL |
| ATOM | 933 | C | LYS | 119 | 47.482 | -5.570 | 19.843 | 1.00 | 18.61 | MTGL |
| ATOM | 934 | O | LYS | 119 | 47.533 | -6.777 | 19.615 | 1.00 | 16.84 | MTGL |
| ATOM | 935 | N | LEU | 120 | 46.339 | -4.911 | 19.975 | 1.00 | 17.54 | MTGL |
| ATOM | 936 | CA | LEU | 120 | 45.064 | -5.599 | 19.820 | 1.00 | 18.74 | MTGL |
| ATOM | 937 | CB | LEU | 120 | 43.909 | -4.643 | 20.144 | 1.00 | 17.57 | MTGL |
| ATOM | 938 | CG | LEU | 120 | 43.736 | -4.330 | 21.635 | 1.00 | 17.26 | MTGL |
| ATOM | 939 | CD1 | LEU | 120 | 42.836 | -3.117 | 21.830 | 1.00 | 17.85 | MTGL |
| ATOM | 940 | CD2 | LEU | 120 | 43.152 | -5.549 | 22.325 | 1.00 | 16.86 | MTGL |
| ATOM | 941 | C | LEU | 120 | 44.976 | -6.086 | 18.372 | 1.00 | 18.39 | MTGL |
| ATOM | 942 | O | LEU | 120 | 44.660 | -7.243 | 18.116 | 1.00 | 19.13 | MTGL |
| ATOM | 943 | N | GLN | 121 | 45.273 | -5.193 | 17.434 | 1.00 | 19.05 | MTGL |
| ATOM | 944 | CA | GLN | 121 | 45.245 | -5.524 | 16.013 | 1.00 | 20.51 | MTGL |
| ATOM | 945 | CB | GLN | 121 | 45.715 | -4.324 | 15.182 | 1.00 | 20.27 | MTGL |
| ATOM | 946 | CG | GLN | 121 | 45.927 | -4.606 | 13.694 | 1.00 | 19.88 | MTGL |
| ATOM | 947 | CD | GLN | 121 | 44.677 | -5.116 | 12.998 | 1.00 | 20.20 | MTGL |
| ATOM | 948 | OE1 | GLN | 121 | 43.565 | -4.680 | 13.291 | 1.00 | 19.32 | MTGL |
| ATOM | 949 | NE2 | GLN | 121 | 44.859 | -6.035 | 12.055 | 1.00 | 20.98 | MTGL |
| ATOM | 950 | C | GLN | 121 | 46.142 | -6.723 | 15.734 | 1.00 | 20.78 | MTGL |
| ATOM | 951 | O | GLN | 121 | 45.729 | -7.672 | 15.078 | 1.00 | 21.20 | MTGL |
| ATOM | 952 | N | ASN | 122 | 47.369 | -6.676 | 16.242 | 1.00 | 20.58 | MTGL |
| ATOM | 953 | CA | ASN | 122 | 48.322 | -7.762 | 16.037 | 1.00 | 22.39 | MTGL |
| ATOM | 954 | CB | ASN | 122 | 49.685 | -7.371 | 16.611 | 1.00 | 24.20 | MTGL |
| ATOM | 955 | CG | ASN | 122 | 50.350 | -6.260 | 15.817 | 1.00 | 26.36 | MTGL |
| ATOM | 956 | OD1 | ASN | 122 | 51.298 | -5.630 | 16.285 | 1.00 | 29.40 | MTGL |
| ATOM | 957 | ND2 | ASN | 122 | 49.863 | -6.021 | 14.605 | 1.00 | 26.25 | MTGL |
| ATOM | 958 | C | ASN | 122 | 47.859 | -9.082 | 16.646 | 1.00 | 22.40 | MTGL |
| ATOM | 959 | O | ASN | 122 | 48.312 | -10.153 | 16.243 | 1.00 | 23.25 | MTGL |
| ATOM | 960 | N | ALA | 123 | 46.957 | -9.005 | 17.616 | 1.00 | 21.34 | MTGL |
| ATOM | 961 | CA | ALA | 123 | 46.436 | -10.209 | 18.252 | 1.00 | 21.19 | MTGL |
| ATOM | 962 | CB | ALA | 123 | 46.151 | -9.939 | 19.730 | 1.00 | 21.28 | MTGL |
| ATOM | 963 | C | ALA | 123 | 45.163 | -10.669 | 17.545 | 1.00 | 20.31 | MTGL |
| ATOM | 964 | O | ALA | 123 | 44.512 | -11.621 | 17.981 | 1.00 | 21.19 | MTGL |
| ATOM | 965 | N | GLY | 124 | 44.813 | -9.985 | 16.457 | 1.00 | 20.00 | MTGL |
| ATOM | 966 | CA | GLY | 124 | 43.621 | -10.332 | 15.705 | 1.00 | 19.34 | MTGL |
| ATOM | 967 | C | GLY | 124 | 42.338 | -9.853 | 16.367 | 1.00 | 20.32 | MTGL |
| ATOM | 968 | O | GLY | 124 | 41.255 | -10.376 | 16.098 | 1.00 | 19.71 | MTGL |
| ATOM | 969 | N | ILE | 125 | 42.450 | -8.855 | 17.239 | 1.00 | 18.85 | MTGL |
| ATOM | 970 | CA | ILE | 125 | 41.281 | -8.327 | 17.928 | 1.00 | 17.97 | MTGL |
| ATOM | 971 | CB | ILE | 125 | 41.502 | -8.279 | 19.465 | 1.00 | 18.21 | MTGL |
| ATOM | 972 | CG2 | ILE | 125 | 40.264 | -7.709 | 20.149 | 1.00 | 18.39 | MTGL |
| ATOM | 973 | CG1 | ILE | 125 | 41.807 | -9.681 | 20.013 | 1.00 | 16.78 | MTGL |
| ATOM | 974 | CD1 | ILE | 125 | 40.682 | -10.694 | 19.808 | 1.00 | 15.33 | MTGL |
| ATOM | 975 | C | ILE | 125 | 40.936 | -6.908 | 17.460 | 1.00 | 18.72 | MTGL |
| ATOM | 976 | O | ILE | 125 | 41.682 | -5.959 | 17.718 | 1.00 | 18.82 | MTGL |
| ATOM | 977 | N | GLN | 126 | 39.810 | -6.771 | 16.769 | 1.00 | 17.38 | MTGL |
| ATOM | 978 | CA | GLN | 126 | 39.355 | -5.463 | 16.310 | 1.00 | 17.54 | MTGL |
| ATOM | 979 | CB | GLN | 126 | 39.059 | -5.459 | 14.810 | 1.00 | 17.95 | MTGL |
| ATOM | 980 | CG | GLN | 126 | 40.267 | -5.634 | 13.905 | 1.00 | 18.48 | MTGL |
| ATOM | 981 | CD | GLN | 126 | 40.704 | -7.082 | 13.784 | 1.00 | 19.41 | MTGL |
| ATOM | 982 | OE1 | GLN | 126 | 39.874 | -7.991 | 13.722 | 1.00 | 18.45 | MTGL |
| ATOM | 983 | NE2 | GLN | 126 | 42.014 | -7.302 | 13.731 | 1.00 | 18.37 | MTGL |
| ATOM | 984 | C | GLN | 126 | 38.078 | -5.152 | 17.073 | 1.00 | 17.01 | MTGL |
| ATOM | 985 | O | GLN | 126 | 36.990 | -5.578 | 16.686 | 1.00 | 17.42 | MTGL |

## Fig. 1 cont.

| ATOM | 986 | N | PRO | 127 | 38.196 | -4.424 | 18.189 | 1.00 | 17.14 | MTGL |
|------|-----|------|-----|-----|--------|--------|--------|------|-------|------|
| ATOM | 987 | CD | PRO | 127 | 39.397 | -3.833 | 18.803 | 1.00 | 16.94 | MTGL |
| ATOM | 988 | CA | PRO | 127 | 36.990 | -4.103 | 18.954 | 1.00 | 17.76 | MTGL |
| ATOM | 989 | CB | PRO | 127 | 37.534 | -3.333 | 20.162 | 1.00 | 17.60 | MTGL |
| ATOM | 990 | CG | PRO | 127 | 38.806 | -2.730 | 19.644 | 1.00 | 20.07 | MTGL |
| ATOM | 991 | C | PRO | 127 | 36.004 | -3.290 | 18.130 | 1.00 | 17.06 | MTGL |
| ATOM | 992 | O | PRO | 127 | 36.400 | -2.472 | 17.303 | 1.00 | 18.03 | MTGL |
| ATOM | 993 | N | THR | 128 | 34.719 | -3.536 | 18.340 | 1.00 | 17.80 | MTGL |
| ATOM | 994 | CA | THR | 128 | 33.688 | -2.803 | 17.620 | 1.00 | 17.59 | MTGL |
| ATOM | 995 | CB | THR | 128 | 32.357 | -3.582 | 17.615 | 1.00 | 18.62 | MTGL |
| ATOM | 996 | OG1 | THR | 128 | 32.035 | -3.994 | 18.951 | 1.00 | 17.44 | MTGL |
| ATOM | 997 | CG2 | THR | 128 | 32.467 | -4.816 | 16.717 | 1.00 | 18.59 | MTGL |
| ATOM | 998 | C | THR | 128 | 33.499 | -1.451 | 18.310 | 1.00 | 17.94 | MTGL |
| ATOM | 999 | O | THR | 128 | 33.086 | -0.476 | 17.683 | 1.00 | 16.71 | MTGL |
| ATOM | 1000 | N | ILE | 129 | 33.834 | -1.397 | 19.600 | 1.00 | 16.54 | MTGL |
| ATOM | 1001 | CA | ILE | 129 | 33.701 | -0.161 | 20.373 | 1.00 | 16.74 | MTGL |
| ATOM | 1002 | CB | ILE | 129 | 32.426 | -0.166 | 21.249 | 1.00 | 17.47 | MTGL |
| ATOM | 1003 | CG2 | ILE | 129 | 32.323 | 1.138 | 22.032 | 1.00 | 16.90 | MTGL |
| ATOM | 1004 | CG1 | ILE | 129 | 31.182 | -0.340 | 20.380 | 1.00 | 18.59 | MTGL |
| ATOM | 1005 | CD1 | ILE | 129 | 29.913 | -0.501 | 21.189 | 1.00 | 18.26 | MTGL |
| ATOM | 1006 | C | ILE | 129 | 34.878 | 0.056 | 21.317 | 1.00 | 16.72 | MTGL |
| ATOM | 1007 | O | ILE | 129 | 35.361 | -0.883 | 21.949 | 1.00 | 16.12 | MTGL |
| ATOM | 1008 | N | VAL | 130 | 35.329 | 1.303 | 21.410 | 1.00 | 16.38 | MTGL |
| ATOM | 1009 | CA | VAL | 130 | 36.413 | 1.666 | 22.313 | 1.00 | 16.43 | MTGL |
| ATOM | 1010 | CB | VAL | 130 | 37.738 | 1.891 | 21.568 | 1.00 | 16.85 | MTGL |
| ATOM | 1011 | CG1 | VAL | 130 | 38.783 | 2.444 | 22.532 | 1.00 | 15.96 | MTGL |
| ATOM | 1012 | CG2 | VAL | 130 | 38.224 | 0.581 | 20.958 | 1.00 | 16.65 | MTGL |
| ATOM | 1013 | C | VAL | 130 | 36.040 | 2.965 | 23.020 | 1.00 | 16.57 | MTGL |
| ATOM | 1014 | O | VAL | 130 | 35.807 | 3.981 | 22.369 | 1.00 | 17.33 | MTGL |
| ATOM | 1015 | N | SER | 131 | 35.955 | 2.931 | 24.347 | 1.00 | 15.26 | MTGL |
| ATOM | 1016 | CA | SER | 131 | 35.640 | 4.142 | 25.088 | 1.00 | 14.32 | MTGL |
| ATOM | 1017 | CB | SER | 131 | 34.741 | 3.840 | 26.296 | 1.00 | 13.74 | MTGL |
| ATOM | 1018 | OG | SER | 131 | 35.427 | 3.100 | 27.299 | 1.00 | 14.55 | MTGL |
| ATOM | 1019 | C | SER | 131 | 36.957 | 4.737 | 25.563 | 1.00 | 13.67 | MTGL |
| ATOM | 1020 | O | SER | 131 | 37.812 | 4.024 | 26.094 | 1.00 | 14.63 | MTGL |
| ATOM | 1021 | N | ILE | 132 | 37.140 | 6.033 | 25.349 | 1.00 | 12.98 | MTGL |
| ATOM | 1022 | CA | ILE | 132 | 38.362 | 6.684 | 25.791 | 1.00 | 13.07 | MTGL |
| ATOM | 1023 | CB | ILE | 132 | 38.793 | 7.796 | 24.811 | 1.00 | 13.05 | MTGL |
| ATOM | 1024 | CG2 | ILE | 132 | 39.419 | 7.169 | 23.573 | 1.00 | 14.24 | MTGL |
| ATOM | 1025 | CG1 | ILE | 132 | 37.591 | 8.649 | 24.397 | 1.00 | 13.32 | MTGL |
| ATOM | 1026 | CD1 | ILE | 132 | 37.960 | 9.760 | 23.429 | 1.00 | 14.06 | MTGL |
| ATOM | 1027 | C | ILE | 132 | 38.103 | 7.234 | 27.188 | 1.00 | 13.33 | MTGL |
| ATOM | 1028 | O | ILE | 132 | 37.800 | 8.415 | 27.372 | 1.00 | 12.93 | MTGL |
| ATOM | 1029 | N | GLY | 133 | 38.206 | 6.339 | 28.170 | 1.00 | 12.78 | MTGL |
| ATOM | 1030 | CA | GLY | 133 | 37.957 | 6.703 | 29.552 | 1.00 | 13.26 | MTGL |
| ATOM | 1031 | C | GLY | 133 | 36.687 | 6.040 | 30.066 | 1.00 | 14.41 | MTGL |
| ATOM | 1032 | O | GLY | 133 | 35.821 | 5.638 | 29.279 | 1.00 | 14.45 | MTGL |
| ATOM | 1033 | N | ASN | 134 | 36.573 | 5.915 | 31.385 | 1.00 | 14.34 | MTGL |
| ATOM | 1034 | CA | ASN | 134 | 35.393 | 5.311 | 31.995 | 1.00 | 14.81 | MTGL |
| ATOM | 1035 | CB | ASN | 134 | 35.797 | 4.063 | 32.780 | 1.00 | 14.03 | MTGL |
| ATOM | 1036 | CG | ASN | 134 | 34.602 | 3.307 | 33.321 | 1.00 | 15.54 | MTGL |
| ATOM | 1037 | OD1 | ASN | 134 | 33.932 | 2.558 | 32.596 | 1.00 | 14.69 | MTGL |
| ATOM | 1038 | ND2 | ASN | 134 | 34.311 | 3.515 | 34.599 | 1.00 | 13.31 | MTGL |
| ATOM | 1039 | C | ASN | 134 | 34.727 | 6.328 | 32.929 | 1.00 | 15.45 | MTGL |
| ATOM | 1040 | O | ASN | 134 | 35.355 | 6.823 | 33.865 | 1.00 | 14.99 | MTGL |
| ATOM | 1041 | N | GLU | 135 | 33.458 | 6.632 | 32.672 | 1.00 | 15.32 | MTGL |
| ATOM | 1042 | CA | GLU | 135 | 32.708 | 7.600 | 33.480 | 1.00 | 16.19 | MTGL |
| ATOM | 1043 | CB | GLU | 135 | 32.225 | 6.948 | 34.780 | 1.00 | 16.84 | MTGL |

Fig. 1 cont.

| ATOM | 1044 | CG  | GLU | 135 | 31.360 | 5.710  | 34.571 | 1.00 | 18.65 | MTGL |
|------|------|-----|-----|-----|--------|--------|--------|------|-------|------|
| ATOM | 1045 | CD  | GLU | 135 | 30.758 | 5.173  | 35.862 | 1.00 | 19.18 | MTGL |
| ATOM | 1046 | OE1 | GLU | 135 | 31.449 | 5.200  | 36.905 | 1.00 | 20.99 | MTGL |
| ATOM | 1047 | OE2 | GLU | 135 | 29.602 | 4.705  | 35.829 | 1.00 | 16.99 | MTGL |
| ATOM | 1048 | C   | GLU | 135 | 33.553 | 8.834  | 33.806 | 1.00 | 16.49 | MTGL |
| ATOM | 1049 | O   | GLU | 135 | 33.777 | 9.153  | 34.974 | 1.00 | 15.93 | MTGL |
| ATOM | 1050 | N   | ILE | 136 | 34.004 | 9.536  | 32.770 | 1.00 | 15.57 | MTGL |
| ATOM | 1051 | CA  | ILE | 136 | 34.846 | 10.712 | 32.957 | 1.00 | 16.13 | MTGL |
| ATOM | 1052 | CB  | ILE | 136 | 35.802 | 10.887 | 31.756 | 1.00 | 16.05 | MTGL |
| ATOM | 1053 | CG2 | ILE | 136 | 36.783 | 9.719  | 31.706 | 1.00 | 16.66 | MTGL |
| ATOM | 1054 | CG1 | ILE | 136 | 35.001 | 10.956 | 30.451 | 1.00 | 16.40 | MTGL |
| ATOM | 1055 | CD1 | ILE | 136 | 35.858 | 11.171 | 29.211 | 1.00 | 14.50 | MTGL |
| ATOM | 1056 | C   | ILE | 136 | 34.060 | 12.006 | 33.168 | 1.00 | 16.79 | MTGL |
| ATOM | 1057 | O   | ILE | 136 | 34.457 | 13.067 | 32.697 | 1.00 | 16.67 | MTGL |
| ATOM | 1058 | N   | ARG | 137 | 32.949 | 11.909 | 33.890 | 1.00 | 17.28 | MTGL |
| ATOM | 1059 | CA  | ARG | 137 | 32.099 | 13.057 | 34.170 | 1.00 | 18.25 | MTGL |
| ATOM | 1060 | CB  | ARG | 137 | 30.884 | 12.612 | 34.976 | 1.00 | 20.33 | MTGL |
| ATOM | 1061 | CG  | ARG | 137 | 29.879 | 13.712 | 35.248 | 1.00 | 22.61 | MTGL |
| ATOM | 1062 | CD  | ARG | 137 | 29.087 | 13.370 | 36.487 | 1.00 | 26.40 | MTGL |
| ATOM | 1063 | NE  | ARG | 137 | 29.837 | 13.668 | 37.696 | 1.00 | 28.06 | MTGL |
| ATOM | 1064 | CZ  | ARG | 137 | 29.643 | 13.076 | 38.869 | 1.00 | 28.40 | MTGL |
| ATOM | 1065 | NH1 | ARG | 137 | 28.726 | 12.132 | 39.006 | 1.00 | 27.39 | MTGL |
| ATOM | 1066 | NH2 | ARG | 137 | 30.355 | 13.459 | 39.918 | 1.00 | 30.54 | MTGL |
| ATOM | 1067 | C   | ARG | 137 | 32.849 | 14.145 | 34.937 | 1.00 | 19.12 | MTGL |
| ATOM | 1068 | O   | ARG | 137 | 32.537 | 15.327 | 34.812 | 1.00 | 19.19 | MTGL |
| ATOM | 1069 | N   | ALA | 138 | 33.832 | 13.744 | 35.738 | 1.00 | 17.89 | MTGL |
| ATOM | 1070 | CA  | ALA | 138 | 34.626 | 14.708 | 36.487 | 1.00 | 18.61 | MTGL |
| ATOM | 1071 | CB  | ALA | 138 | 34.679 | 14.320 | 37.965 | 1.00 | 18.89 | MTGL |
| ATOM | 1072 | C   | ALA | 138 | 36.028 | 14.744 | 35.888 | 1.00 | 18.04 | MTGL |
| ATOM | 1073 | O   | ALA | 138 | 37.003 | 15.050 | 36.573 | 1.00 | 18.75 | MTGL |
| ATOM | 1074 | N   | GLY | 139 | 36.119 | 14.415 | 34.603 | 1.00 | 17.60 | MTGL |
| ATOM | 1075 | CA  | GLY | 139 | 37.401 | 14.424 | 33.920 | 1.00 | 16.74 | MTGL |
| ATOM | 1076 | C   | GLY | 139 | 38.141 | 13.103 | 33.979 | 1.00 | 17.00 | MTGL |
| ATOM | 1077 | O   | GLY | 139 | 37.558 | 12.061 | 34.303 | 1.00 | 15.56 | MTGL |
| ATOM | 1078 | N   | LEU | 140 | 39.430 | 13.150 | 33.653 | 1.00 | 16.36 | MTGL |
| ATOM | 1079 | CA  | LEU | 140 | 40.288 | 11.965 | 33.666 | 1.00 | 16.91 | MTGL |
| ATOM | 1080 | CB  | LEU | 140 | 40.254 | 11.255 | 32.308 | 1.00 | 16.55 | MTGL |
| ATOM | 1081 | CG  | LEU | 140 | 40.965 | 11.954 | 31.137 | 1.00 | 17.14 | MTGL |
| ATOM | 1082 | CD1 | LEU | 140 | 41.157 | 10.962 | 29.985 | 1.00 | 17.61 | MTGL |
| ATOM | 1083 | CD2 | LEU | 140 | 40.158 | 13.157 | 30.673 | 1.00 | 16.51 | MTGL |
| ATOM | 1084 | C   | LEU | 140 | 41.731 | 12.366 | 33.961 | 1.00 | 16.82 | MTGL |
| ATOM | 1085 | O   | LEU | 140 | 42.078 | 13.549 | 33.919 | 1.00 | 16.86 | MTGL |
| ATOM | 1086 | N   | LEU | 141 | 42.566 | 11.373 | 34.254 | 1.00 | 16.21 | MTGL |
| ATOM | 1087 | CA  | LEU | 141 | 43.979 | 11.616 | 34.521 | 1.00 | 16.03 | MTGL |
| ATOM | 1088 | CB  | LEU | 141 | 44.711 | 11.839 | 33.191 | 1.00 | 14.81 | MTGL |
| ATOM | 1089 | CG  | LEU | 141 | 44.626 | 10.646 | 32.220 | 1.00 | 15.72 | MTGL |
| ATOM | 1090 | CD1 | LEU | 141 | 45.076 | 11.054 | 30.818 | 1.00 | 14.73 | MTGL |
| ATOM | 1091 | CD2 | LEU | 141 | 45.494 | 9.501  | 32.752 | 1.00 | 14.97 | MTGL |
| ATOM | 1092 | C   | LEU | 141 | 44.166 | 12.822 | 35.444 | 1.00 | 16.13 | MTGL |
| ATOM | 1093 | O   | LEU | 141 | 44.776 | 13.819 | 35.069 | 1.00 | 15.77 | MTGL |
| ATOM | 1094 | N   | TRP | 142 | 43.631 | 12.715 | 36.655 | 1.00 | 16.15 | MTGL |
| ATOM | 1095 | CA  | TRP | 142 | 43.718 | 13.789 | 37.635 | 1.00 | 16.13 | MTGL |
| ATOM | 1096 | CB  | TRP | 142 | 42.854 | 13.446 | 38.845 | 1.00 | 16.04 | MTGL |
| ATOM | 1097 | CG  | TRP | 142 | 41.387 | 13.408 | 38.559 | 1.00 | 16.68 | MTGL |
| ATOM | 1098 | CD2 | TRP | 142 | 40.345 | 13.114 | 39.494 | 1.00 | 16.86 | MTGL |
| ATOM | 1099 | CE2 | TRP | 142 | 39.117 | 13.217 | 38.800 | 1.00 | 16.85 | MTGL |
| ATOM | 1100 | CE3 | TRP | 142 | 40.330 | 12.779 | 40.855 | 1.00 | 17.53 | MTGL |
| ATOM | 1101 | CD1 | TRP | 142 | 40.769 | 13.669 | 37.365 | 1.00 | 16.02 | MTGL |

# Fig. 1 cont.

| ATOM | 1102 | NE1 | TRP | 142 | 39.404 | 13.557 | 37.503 | 1.00 | 16.14 | MTGL |
| ATOM | 1103 | CZ2 | TRP | 142 | 37.884 | 12.993 | 39.421 | 1.00 | 16.71 | MTGL |
| ATOM | 1104 | CZ3 | TRP | 142 | 39.097 | 12.557 | 41.475 | 1.00 | 17.85 | MTGL |
| ATOM | 1105 | CH2 | TRP | 142 | 37.894 | 12.666 | 40.755 | 1.00 | 17.70 | MTGL |
| ATOM | 1106 | C | TRP | 142 | 45.151 | 14.036 | 38.092 | 1.00 | 16.70 | MTGL |
| ATOM | 1107 | O | TRP | 142 | 45.965 | 13.116 | 38.132 | 1.00 | 15.98 | MTGL |
| ATOM | 1108 | N | PRO | 143 | 45.476 | 15.289 | 38.452 | 1.00 | 18.10 | MTGL |
| ATOM | 1109 | CD | PRO | 143 | 46.716 | 15.597 | 39.183 | 1.00 | 18.05 | MTGL |
| ATOM | 1110 | CA | PRO | 143 | 44.586 | 16.458 | 38.444 | 1.00 | 17.24 | MTGL |
| ATOM | 1111 | CB | PRO | 143 | 45.170 | 17.362 | 39.539 | 1.00 | 17.56 | MTGL |
| ATOM | 1112 | CG | PRO | 143 | 46.199 | 16.496 | 40.260 | 1.00 | 19.44 | MTGL |
| ATOM | 1113 | C | PRO | 143 | 44.599 | 17.177 | 37.096 | 1.00 | 17.09 | MTGL |
| ATOM | 1114 | O | PRO | 143 | 43.804 | 18.092 | 36.864 | 1.00 | 16.74 | MTGL |
| ATOM | 1115 | N | THR | 144 | 45.509 | 16.767 | 36.219 | 1.00 | 16.23 | MTGL |
| ATOM | 1116 | CA | THR | 144 | 45.651 | 17.396 | 34.910 | 1.00 | 17.05 | MTGL |
| ATOM | 1117 | CB | THR | 144 | 46.677 | 16.640 | 34.048 | 1.00 | 17.49 | MTGL |
| ATOM | 1118 | OG1 | THR | 144 | 47.864 | 16.413 | 34.817 | 1.00 | 18.41 | MTGL |
| ATOM | 1119 | CG2 | THR | 144 | 47.040 | 17.453 | 32.811 | 1.00 | 17.61 | MTGL |
| ATOM | 1120 | C | THR | 144 | 44.346 | 17.510 | 34.129 | 1.00 | 16.98 | MTGL |
| ATOM | 1121 | O | THR | 144 | 44.027 | 18.579 | 33.610 | 1.00 | 17.37 | MTGL |
| ATOM | 1122 | N | GLY | 145 | 43.594 | 16.414 | 34.052 | 1.00 | 17.00 | MTGL |
| ATOM | 1123 | CA | GLY | 145 | 42.336 | 16.432 | 33.322 | 1.00 | 16.55 | MTGL |
| ATOM | 1124 | C | GLY | 145 | 41.111 | 16.472 | 34.219 | 1.00 | 17.19 | MTGL |
| ATOM | 1125 | O | GLY. | 145 | 40.033 | 16.013 | 33.837 | 1.00 | 15.11 | MTGL |
| ATOM | 1126 | N | ARG | 146 | 41.269 | 17.009 | 35.423 | 1.00 | 16.86 | MTGL |
| ATOM | 1127 | CA | ARG | 146 | 40.153 | 17.118 | 36.361 | 1.00 | 18.80 | MTGL |
| ATOM | 1128 | CB | ARG | 146 | 40.707 | 17.308 | 37.784 | 1.00 | 20.43 | MTGL |
| ATOM | 1129 | CG | ARG | 146 | 39.671 | 17.572 | 38.870 | 1.00 | 24.77 | MTGL |
| ATOM | 1130 | CD | ARG | 146 | 38.729 | 16.394 | 39.052 | 1.00 | 27.03 | MTGL |
| ATOM | 1131 | NE | ARG | 146 | 37.715 | 16.623 | 40.081 | 1.00 | 30.10 | MTGL |
| ATOM | 1132 | CZ | ARG | 146 | 37.922 | 16.516 | 41.391 | 1.00 | 31.39 | MTGL |
| ATOM | 1133 | NH1 | ARG | 146 | 39.122 | 16.182 | 41.861 | 1.00 | 31.38 | MTGL |
| ATOM | 1134 | NH2 | ARG | 146 | 36.916 | 16.729 | 42.236 | 1.00 | 32.17 | MTGL |
| ATOM | 1135 | C | ARG | 146 | 39.261 | 18.308 | 35.961 | 1.00 | 18.91 | MTGL |
| ATOM | 1136 | O | ARG | 146 | 39.763 | 19.344 | 35.534 | 1.00 | 17.30 | MTGL |
| ATOM | 1137 | N | THR | 147 | 37.940 | 18.147 | 36.055 | 1.00 | 18.95 | MTGL |
| ATOM | 1138 | CA | THR | 147 | 37.037 | 19.255 | 35.732 | 1.00 | 19.02 | MTGL |
| ATOM | 1139 | CB | THR | 147 | 35.550 | 18.826 | 35.731 | 1.00 | 18.33 | MTGL |
| ATOM | 1140 | OG1 | THR | 147 | 35.278 | 18.044 | 36.890 | 1.00 | 18.17 | MTGL |
| ATOM | 1141 | CG2 | THR | 147 | 35.217 | 18.016 | 34.490 | 1.00 | 18.17 | MTGL |
| ATOM | 1142 | C | THR | 147 | 37.278 | 20.271 | 36.858 | 1.00 | 19.51 | MTGL |
| ATOM | 1143 | O | THR | 147 | 37.539 | 19.861 | 37.983 | 1.00 | 18.48 | MTGL |
| ATOM | 1144 | N | GLU | 148 | 37.158 | 21.574 | 36.598 | 1.00 | 19.44 | MTGL |
| ATOM | 1145 | CA | GLU | 148 | 36.771 | 22.124 | 35.317 | 1.00 | 20.37 | MTGL |
| ATOM | 1146 | CB | GLU | 148 | 35.829 | 23.309 | 35.551 | 1.00 | 22.32 | MTGL |
| ATOM | 1147 | CG | GLU | 148 | 34.576 | 22.960 | 36.356 | 1.00 | 26.58 | MTGL |
| ATOM | 1148 | CD | GLU | 148 | 34.081 | 24.123 | 37.217 | 1.00 | 29.48 | MTGL |
| ATOM | 1149 | OE1 | GLU | 148 | 33.777 | 25.209 | 36.672 | 1.00 | 30.90 | MTGL |
| ATOM | 1150 | OE2 | GLU | 148 | 33.988 | 23.929 | 38.448 | 1.00 | 30.75 | MTGL |
| ATOM | 1151 | C | GLU | 148 | 37.858 | 22.540 | 34.312 | 1.00 | 20.17 | MTGL |
| ATOM | 1152 | O | GLU | 148 | 37.649 | 23.550 | 33.633 | 1.00 | 20.26 | MTGL |
| ATOM | 1153 | N | ASN | 149 | 39.019 | 21.853 | 34.186 | 0.50 | 20.18 | MTGL |
| ATOM | 1154 | CA | ASN | 149 | 40.039 | 22.216 | 33.154 | 0.50 | 20.26 | MTGL |
| ATOM | 1155 | CB | ASN | 149 | 41.436 | 21.616 | 33.436 | 0.50 | 21.36 | MTGL |
| ATOM | 1156 | CG | ASN | 149 | 42.198 | 22.423 | 34.433 | 0.50 | 22.41 | MTGL |
| ATOM | 1157 | OD1 | ASN | 149 | 42.651 | 23.520 | 34.132 | 0.50 | 23.31 | MTGL |
| ATOM | 1158 | ND2 | ASN | 149 | 42.298 | 21.917 | 35.646 | 0.50 | 23.40 | MTGL |
| ATOM | 1159 | C | ASN | 149 | 39.555 | 21.656 | 31.811 | 0.50 | 19.48 | MTGL |

Fig. 1 cont.

| ATOM | 1160 | O | ASN | 149 | 40.152 | 20.702 | 31.289 | 0.50 | 17.94 | MTGL |
|------|------|-----|-----|-----|--------|--------|--------|------|-------|------|
| ATOM | 1161 | N | TRP | 150 | 38.480 | 22.230 | 31.261 | 1.00 | 19.00 | MTGL |
| ATOM | 1162 | CA | TRP | 150 | 37.920 | 21.769 | 30.000 | 1.00 | 18.91 | MTGL |
| ATOM | 1163 | CB | TRP | 150 | 36.777 | 22.704 | 29.605 | 1.00 | 18.17 | MTGL |
| ATOM | 1164 | CG | TRP | 150 | 35.710 | 22.781 | 30.629 | 1.00 | 17.82 | MTGL |
| ATOM | 1165 | CD2 | TRP | 150 | 34.895 | 21.702 | 31.094 | 1.00 | 18.44 | MTGL |
| ATOM | 1166 | CE2 | TRP | 150 | 34.013 | 22.232 | 32.060 | 1.00 | 18.24 | MTGL |
| ATOM | 1167 | CE3 | TRP | 150 | 34.824 | 20.335 | 30.787 | 1.00 | 18.25 | MTGL |
| ATOM | 1168 | CD1 | TRP | 150 | 35.301 | 23.895 | 31.310 | 1.00 | 17.99 | MTGL |
| ATOM | 1169 | NE1 | TRP | 150 | 34.282 | 23.571 | 32.170 | 1.00 | 19.19 | MTGL |
| ATOM | 1170 | CZ2 | TRP | 150 | 33.066 | 21.443 | 32.725 | 1.00 | 19.86 | MTGL |
| ATOM | 1171 | CZ3 | TRP | 150 | 33.879 | 19.547 | 31.448 | 1.00 | 19.02 | MTGL |
| ATOM | 1172 | CH2 | TRP | 150 | 33.013 | 20.105 | 32.408 | 1.00 | 19.52 | MTGL |
| ATOM | 1173 | C | TRP | 150 | 38.990 | 21.744 | 28.904 | 1.00 | 19.25 | MTGL |
| ATOM | 1174 | O | TRP | 150 | 39.022 | 20.828 | 28.091 | 1.00 | 19.43 | MTGL |
| ATOM | 1175 | N | ALA | 151 | 39.851 | 22.759 | 28.880 | 1.00 | 17.86 | MTGL |
| ATOM | 1176 | CA | ALA | 151 | 40.897 | 22.822 | 27.864 | 1.00 | 18.96 | MTGL |
| ATOM | 1177 | CB | ALA | 151 | 41.753 | 24.090 | 28.047 | 1.00 | 19.41 | MTGL |
| ATOM | 1178 | C | ALA | 151 | 41.784 | 21.571 | 27.897 | 1.00 | 18.90 | MTGL |
| ATOM | 1179 | O | ALA | 151 | 42.098 | 20.994 | 26.857 | 1.00 | 19.89 | MTGL |
| ATOM | 1180 | N | ASN | 152 | 42.184 | 21.144 | 29.088 | 1.00 | 18.45 | MTGL |
| ATOM | 1181 | CA | ASN | 152 | 43.027 | 19.954 | 29.209 | 1.00 | 18.07 | MTGL |
| ATOM | 1182 | CB | ASN | 152 | 43.584 | 19.830 | 30.635 | 1.00 | 16.97 | MTGL |
| ATOM | 1183 | CG | ASN | 152 | 44.767 | 20.764 | 30.886 | 1.00 | 18.19 | MTGL |
| ATOM | 1184 | OD1 | ASN | 152 | 45.095 | 21.603 | 30.054 | 1.00 | 17.89 | MTGL |
| ATOM | 1185 | ND2 | ASN | 152 | 45.407 | 20.618 | 32.043 | 1.00 | 17.33 | MTGL |
| ATOM | 1186 | C | ASN | 152 | 42.250 | 18.686 | 28.848 | 1.00 | 17.48 | MTGL |
| ATOM | 1187 | O | ASN | 152 | 42.762 | 17.805 | 28.155 | 1.00 | 17.16 | MTGL |
| ATOM | 1188 | N | ILE | 153 | 41.016 | 18.598 | 29.325 | 1.00 | 17.57 | MTGL |
| ATOM | 1189 | CA | ILE | 153 | 40.177 | 17.437 | 29.048 | 1.00 | 18.34 | MTGL |
| ATOM | 1190 | CB | ILE | 153 | 38.801 | 17.573 | 29.741 | 1.00 | 17.84 | MTGL |
| ATOM | 1191 | CG2 | ILE | 153 | 37.836 | 16.486 | 29.243 | 1.00 | 17.51 | MTGL |
| ATOM | 1192 | CG1 | ILE | 153 | 38.987 | 17.468 | 31.255 | 1.00 | 17.49 | MTGL |
| ATOM | 1193 | CD1 | ILE | 153 | 37.761 | 17.837 | 32.060 | 1.00 | 17.26 | MTGL |
| ATOM | 1194 | C | ILE | 153 | 39.974 | 17.246 | 27.548 | 1.00 | 17.82 | MTGL |
| ATOM | 1195 | O | ILE | 153 | 40.174 | 16.150 | 27.027 | 1.00 | 17.52 | MTGL |
| ATOM | 1196 | N | ALA | 154 | 39.596 | 18.318 | 26.858 | 1.00 | 17.93 | MTGL |
| ATOM | 1197 | CA | ALA | 154 | 39.359 | 18.255 | 25.416 | 1.00 | 18.68 | MTGL |
| ATOM | 1198 | CB | ALA | 154 | 38.884 | 19.620 | 24.896 | 1.00 | 17.82 | MTGL |
| ATOM | 1199 | C | ALA | 154 | 40.624 | 17.834 | 24.686 | 1.00 | 18.79 | MTGL |
| ATOM | 1200 | O | ALA | 154 | 40.584 | 17.037 | 23.744 | 1.00 | 17.95 | MTGL |
| ATOM | 1201 | N | ARG | 155 | 41.749 | 18.375 | 25.131 | 1.00 | 18.32 | MTGL |
| ATÓM | 1202 | CA | ARG | 155 | 43.025 | 18.064 | 24.512 | 1.00 | 19.09 | MTGL |
| ATOM | 1203 | CB | ARG | 155 | 44.098 | 18.972 | 25.094 | 1.00 | 20.03 | MTGL |
| ATOM | 1204 | CG | ARG | 155 | 45.415 | 18.867 | 24.403 | 1.00 | 23.57 | MTGL |
| ATOM | 1205 | CD | ARG | 155 | 46.295 | 19.990 | 24.873 | 1.00 | 26.84 | MTGL |
| ATOM | 1206 | NE | ARG | 155 | 47.681 | 19.767 | 24.498 | 1.00 | 29.65 | MTGL |
| ATOM | 1207 | CZ | ARG | 155 | 48.686 | 20.513 | 24.931 | 1.00 | 28.58 | MTGL |
| ATOM | 1208 | NH1 | ARG | 155 | 48.443 | 21.525 | 25.753 | 1.00 | 29.23 | MTGL |
| ATOM | 1209 | NH2 | ARG | 155 | 49.922 | 20.244 | 24.540 | 1.00 | 29.12 | MTGL |
| ATOM | 1210 | C | ARG | 155 | 43.402 | 16.598 | 24.721 | 1.00 | 18.37 | MTGL |
| ATOM | 1211 | O | ARG | 155 | 43.848 | 15.916 | 23.792 | 1.00 | 17.92 | MTGL |
| ATOM | 1212 | N | LEU | 156 | 43.217 | 16.115 | 25.944 | 1.00 | 17.77 | MTGL |
| ATOM | 1213 | CA | LEU | 156 | 43.540 | 14.731 | 26.258 | 1.00 | 17.18 | MTGL |
| ATOM | 1214 | CB | LEU | 156 | 43.360 | 14.473 | 27.761 | 1.00 | 16.68 | MTGL |
| ATOM | 1215 | CG | LEU | 156 | 44.375 | 15.158 | 28.689 | 1.00 | 16.04 | MTGL |
| ATOM | 1216 | CD1 | LEU | 156 | 43.921 | 15.032 | 30.139 | 1.00 | 17.64 | MTGL |
| ATOM | 1217 | CD2 | LEU | 156 | 45.745 | 14.532 | 28.504 | 1.00 | 14.11 | MTGL |

## Fig. 1 cont.

| ATOM | 1218 | C   | LEU | 156 | 42.660 | 13.777 | 25.447 | 1.00 | 17.29 | MTGL |
|------|------|-----|-----|-----|--------|--------|--------|------|-------|------|
| ATOM | 1219 | O   | LEU | 156 | 43.152 | 12.794 | 24.886 | 1.00 | 16.71 | MTGL |
| ATOM | 1220 | N   | LEU | 157 | 41.363 | 14.071 | 25.377 | 1.00 | 16.48 | MTGL |
| ATOM | 1221 | CA  | LEU | 157 | 40.438 | 13.219 | 24.639 | 1.00 | 16.71 | MTGL |
| ATOM | 1222 | CB  | LEU | 157 | 38.992 | 13.651 | 24.900 | 1.00 | 15.25 | MTGL |
| ATOM | 1223 | CG  | LEU | 157 | 38.509 | 13.425 | 26.339 | 1.00 | 14.15 | MTGL |
| ATOM | 1224 | CD1 | LEU | 157 | 37.080 | 13.903 | 26.505 | 1.00 | 13.65 | MTGL |
| ATOM | 1225 | CD2 | LEU | 157 | 38.599 | 11.944 | 26.676 | 1.00 | 13.61 | MTGL |
| ATOM | 1226 | C   | LEU | 157 | 40.744 | 13.230 | 23.146 | 1.00 | 18.12 | MTGL |
| ATOM | 1227 | O   | LEU | 157 | 40.549 | 12.224 | 22.456 | 1.00 | 16.85 | MTGL |
| ATOM | 1228 | N   | HIS | 158 | 41.231 | 14.366 | 22.652 | 1.00 | 19.80 | MTGL |
| ATOM | 1229 | CA  | HIS | 158 | 41.600 | 14.498 | 21.244 | 1.00 | 20.98 | MTGL |
| ATOM | 1230 | CB  | HIS | 158 | 42.001 | 15.946 | 20.938 | 1.00 | 22.94 | MTGL |
| ATOM | 1231 | CG  | HIS | 158 | 42.458 | 16.170 | 19.528 | 1.00 | 24.32 | MTGL |
| ATOM | 1232 | CD2 | HIS | 158 | 43.695 | 16.367 | 19.013 | 1.00 | 23.88 | MTGL |
| ATOM | 1233 | ND1 | HIS | 158 | 41.586 | 16.230 | 18.460 | 1.00 | 24.92 | MTGL |
| ATOM | 1234 | CE1 | HIS | 158 | 42.266 | 16.460 | 17.350 | 1.00 | 23.22 | MTGL |
| ATOM | 1235 | NE2 | HIS | 158 | 43.548 | 16.547 | 17.658 | 1.00 | 24.57 | MTGL |
| ATOM | 1236 | C   | HIS | 158 | 42.783 | 13.567 | 20.973 | 1.00 | 21.01 | MTGL |
| ATOM | 1237 | O   | HIS | 158 | 42.809 | 12.851 | 19.971 | 1.00 | 21.78 | MTGL |
| ATOM | 1238 | N   | SER | 159 | 43.762 | 13.578 | 21.874 | 1.00 | 20.28 | MTGL |
| ATOM | 1239 | CA  | SER | 159 | 44.940 | 12.730 | 21.726 | 1.00 | 20.15 | MTGL |
| ATOM | 1240 | CB  | SER | 159 | 45.961 | 13.021 | 22.829 | 1.00 | 21.81 | MTGL |
| ATOM | 1241 | OG  | SER | 159 | 46.476 | 14.333 | 22.721 | 1.00 | 24.73 | MTGL |
| ATOM | 1242 | C   | SER | 159 | 44.570 | 11.253 | 21.774 | 1.00 | 18.92 | MTGL |
| ATOM | 1243 | O   | SER | 159 | 45.095 | 10.453 | 21.004 | 1.00 | 19.31 | MTGL |
| ATOM | 1244 | N   | ALA | 160 | 43.675 | 10.894 | 22.687 | 1.00 | 17.87 | MTGL |
| ATOM | 1245 | CA  | ALA | 160 | 43.249 | 9.504  | 22.824 | 1.00 | 17.96 | MTGL |
| ATOM | 1246 | CB  | ALA | 160 | 42.322 | 9.352  | 24.026 | 1.00 | 18.26 | MTGL |
| ATOM | 1247 | C   | ALA | 160 | 42.538 | 9.044  | 21.556 | 1.00 | 18.59 | MTGL |
| ATOM | 1248 | O   | ALA | 160 | 42.844 | 7.982  | 21.013 | 1.00 | 17.77 | MTGL |
| ATOM | 1249 | N   | ALA | 161 | 41.593 | 9.852  | 21.083 | 1.00 | 18.03 | MTGL |
| ATOM | 1250 | CA  | ALA | 161 | 40.846 | 9.519  | 19.875 | 1.00 | 18.84 | MTGL |
| ATOM | 1251 | CB  | ALA | 161 | 39.851 | 10.623 | 19.547 | 1.00 | 16.85 | MTGL |
| ATOM | 1252 | C   | ALA | 161 | 41.778 | 9.294  | 18.695 | 1.00 | 18.82 | MTGL |
| ATOM | 1253 | O   | ALA | 161 | 41.654 | 8.301  | 17.983 | 1.00 | 19.53 | MTGL |
| ATOM | 1254 | N   | TRP | 162 | 42.715 | 10.211 | 18.485 | 1.00 | 18.98 | MTGL |
| ATOM | 1255 | CA  | TRP | 162 | 43.636 | 10.057 | 17.371 | 1.00 | 19.92 | MTGL |
| ATOM | 1256 | CB  | TRP | 162 | 44.330 | 11.386 | 17.064 | 1.00 | 21.12 | MTGL |
| ATOM | 1257 | CG  | TRP | 162 | 43.420 | 12.264 | 16.268 | 1.00 | 24.00 | MTGL |
| ATOM | 1258 | CD2 | TRP | 162 | 43.215 | 12.212 | 14.851 | 1.00 | 24.55 | MTGL |
| ATOM | 1259 | CE2 | TRP | 162 | 42.158 | 13.102 | 14.546 | 1.00 | 24.96 | MTGL |
| ATOM | 1260 | CE3 | TRP | 162 | 43.822 | 11.499 | 13.808 | 1.00 | 25.38 | MTGL |
| ATOM | 1261 | CD1 | TRP | 162 | 42.509 | 13.160 | 16.752 | 1.00 | 24.55 | MTGL |
| ATOM | 1262 | NE1 | TRP | 162 | 41.743 | 13.665 | 15.724 | 1.00 | 25.20 | MTGL |
| ATOM | 1263 | CZ2 | TRP | 162 | 41.691 | 13.293 | 13.241 | 1.00 | 24.56 | MTGL |
| ATOM | 1264 | CZ3 | TRP | 162 | 43.355 | 11.689 | 12.507 | 1.00 | 25.72 | MTGL |
| ATOM | 1265 | CH2 | TRP | 162 | 42.302 | 12.581 | 12.238 | 1.00 | 24.73 | MTGL |
| ATOM | 1266 | C   | TRP | 162 | 44.643 | 8.927  | 17.556 | 1.00 | 20.10 | MTGL |
| ATOM | 1267 | O   | TRP | 162 | 45.263 | 8.483  | 16.596 | 1.00 | 19.99 | MTGL |
| ATOM | 1268 | N   | GLY | 163 | 44.803 | 8.458  | 18.786 | 1.00 | 20.69 | MTGL |
| ATOM | 1269 | CA  | GLY | 163 | 45.703 | 7.343  | 19.016 | 1.00 | 20.86 | MTGL |
| ATOM | 1270 | C   | GLY | 163 | 45.051 | 6.124  | 18.375 | 1.00 | 20.81 | MTGL |
| ATOM | 1271 | O   | GLY | 163 | 45.720 | 5.225  | 17.868 | 1.00 | 20.64 | MTGL |
| ATOM | 1272 | N   | ILE | 164 | 43.724 | 6.109  | 18.395 | 1.00 | 20.00 | MTGL |
| ATOM | 1273 | CA  | ILE | 164 | 42.956 | 5.020  | 17.810 | 1.00 | 19.28 | MTGL |
| ATOM | 1274 | CB  | ILE | 164 | 41.515 | 5.020  | 18.347 | 1.00 | 18.69 | MTGL |
| ATOM | 1275 | CG2 | ILE | 164 | 40.670 | 3.977  | 17.601 | 1.00 | 17.15 | MTGL |

# Fig. 1 cont.

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1276 | CG1 | ILE | 164 | 41.529 | 4.750 | 19.852 | 1.00 | 18.11 | MTGL |
| ATOM | 1277 | CD1 | ILE | 164 | 40.155 | 4.779 | 20.489 | 1.00 | 18.52 | MTGL |
| ATOM | 1278 | C | ILE | 164 | 42.913 | 5.181 | 16.291 | 1.00 | 20.20 | MTGL |
| ATOM | 1279 | O | ILE | 164 | 43.125 | 4.219 | 15.548 | 1.00 | 18.00 | MTGL |
| ATOM | 1280 | N | LYS | 165 | 42.645 | 6.405 | 15.839 | 1.00 | 20.30 | MTGL |
| ATOM | 1281 | CA | LYS | 165 | 42.563 | 6.701 | 14.410 | 1.00 | 21.80 | MTGL |
| ATOM | 1282 | CB | LYS | 165 | 42.100 | 8.149 | 14.191 | 1.00 | 21.88 | MTGL |
| ATOM | 1283 | CG | LYS | 165 | 40.670 | 8.436 | 14.647 | 1.00 | 23.28 | MTGL |
| ATOM | 1284 | CD | LYS | 165 | 40.346 | 9.924 | 14.509 | 1.00 | 22.94 | MTGL |
| ATOM | 1285 | CE | LYS | 165 | 38.989 | 10.268 | 15.097 | 1.00 | 24.34 | MTGL |
| ATOM | 1286 | NZ | LYS | 165 | 37.857 | 9.632 | 14.363 | 1.00 | 25.77 | MTGL |
| ATOM | 1287 | C | LYS | 165 | 43.879 | 6.468 | 13.668 | 1.00 | 21.72 | MTGL |
| ATOM | 1288 | O | LYS | 165 | 43.868 | 6.086 | 12.501 | 1.00 | 21.82 | MTGL |
| ATOM | 1289 | N | ASP | 166 | 45.009 | 6.699 | 14.335 | 1.00 | 22.15 | MTGL |
| ATOM | 1290 | CA | ASP | 166 | 46.315 | 6.496 | 13.705 | 1.00 | 21.98 | MTGL |
| ATOM | 1291 | CB | ASP | 166 | 47.373 | 7.438 | 14.299 | 1.00 | 22.61 | MTGL |
| ATOM | 1292 | CG | ASP | 166 | 47.119 | 8.907 | 13.970 | 1.00 | 24.69 | MTGL |
| ATOM | 1293 | OD1 | ASP | 166 | 46.345 | 9.197 | 13.032 | 1.00 | 25.51 | MTGL |
| ATOM | 1294 | OD2 | ASP | 166 | 47.709 | 9.775 | 14.645 | 1.00 | 23.73 | MTGL |
| ATOM | 1295 | C | ASP | 166 | 46.818 | 5.063 | 13.853 | 1.00 | 21.80 | MTGL |
| ATOM | 1296 | O | ASP | 166 | 47.900 | 4.737 | 13.373 | 1.00 | 22.35 | MTGL |
| ATOM | 1297 | N | SER | 167 | 46.043 | 4.208 | 14.511 | 1.00 | 21.58 | MTGL |
| ATOM | 1298 | CA | SER | 167 | 46.460 | 2.822 | 14.722 | 1.00 | 21.57 | MTGL |
| ATOM | 1299 | CB | SER | 167 | 45.724 | 2.229 | 15.927 | 1.00 | 20.98 | MTGL |
| ATOM | 1300 | OG | SER | 167 | 44.368 | 1.952 | 15.620 | 1.00 | 20.07 | MTGL |
| ATOM | 1301 | C | SER | 167 | 46.235 | 1.920 | 13.508 | 1.00 | 21.73 | MTGL |
| ATOM | 1302 | O | SER | 167 | 45.669 | 2.347 | 12.503 | 1.00 | 21.01 | MTGL |
| ATOM | 1303 | N | SER | 168 | 46.676 | 0.668 | 13.619 | 1.00 | 21.44 | MTGL |
| ATOM | 1304 | CA | SER | 168 | 46.520 | -0.304 | 12.539 | 1.00 | 20.71 | MTGL |
| ATOM | 1305 | CB | SER | 168 | 47.711 | -1.264 | 12.519 | 1.00 | 21.31 | MTGL |
| ATOM | 1306 | OG | SER | 168 | 47.836 | -1.921 | 13.768 | 1.00 | 23.08 | MTGL |
| ATOM | 1307 | C | SER | 168 | 45.229 | -1.116 | 12.654 | 1.00 | 20.14 | MTGL |
| ATOM | 1308 | O | SER | 168 | 45.001 | -2.033 | 11.869 | 1.00 | 19.79 | MTGL |
| ATOM | 1309 | N | LEU | 169 | 44.388 | -0.792 | 13.630 | 1.00 | 19.27 | MTGL |
| ATOM | 1310 | CA | LEU | 169 | 43.132 | -1.514 | 13.791 | 1.00 | 19.92 | MTGL |
| ATOM | 1311 | CB | LEU | 169 | 42.306 | -0.921 | 14.935 | 1.00 | 19.48 | MTGL |
| ATOM | 1312 | CG | LEU | 169 | 42.758 | -1.226 | 16.365 | 1.00 | 19.56 | MTGL |
| ATOM | 1313 | CD1 | LEU | 169 | 41.918 | -0.417 | 17.342 | 1.00 | 18.93 | MTGL |
| ATOM | 1314 | CD2 | LEU | 169 | 42.612 | -2.717 | 16.650 | 1.00 | 19.30 | MTGL |
| ATOM | 1315 | C | LEU | 169 | 42.323 | -1.450 | 12.501 | 1.00 | 20.54 | MTGL |
| ATOM | 1316 | O | LEU | 169 | 42.053 | -0.365 | 11.981 | 1.00 | 20.27 | MTGL |
| ATOM | 1317 | N | SER | 170 | 41.940 | -2.614 | 11.987 | 1.00 | 20.36 | MTGL |
| ATOM | 1318 | CA | SER | 170 | 41.159 | -2.678 | 10.760 | 1.00 | 21.47 | MTGL |
| ATOM | 1319 | CB | SER | 170 | 42.088 | -2.784 | 9.545 | 1.00 | 22.54 | MTGL |
| ATOM | 1320 | OG | SER | 170 | 41.344 | -2.749 | 8.341 | 1.00 | 22.78 | MTGL |
| ATOM | 1321 | C | SER | 170 | 40.216 | -3.875 | 10.797 | 1.00 | 21.69 | MTGL |
| ATOM | 1322 | O | SER | 170 | 40.659 | -5.024 | 10.819 | 1.00 | 21.79 | MTGL |
| ATOM | 1323 | N | PRO | 171 | 38.899 | -3.621 | 10.800 | 1.00 | 21.30 | MTGL |
| ATOM | 1324 | CD | PRO | 171 | 37.874 | -4.676 | 10.884 | 1.00 | 21.70 | MTGL |
| ATOM | 1325 | CA | PRO | 171 | 38.277 | -2.294 | 10.764 | 1.00 | 21.48 | MTGL |
| ATOM | 1326 | CB | PRO | 171 | 36.806 | -2.616 | 10.530 | 1.00 | 21.60 | MTGL |
| ATOM | 1327 | CG | PRO | 171 | 36.644 | -3.901 | 11.285 | 1.00 | 22.67 | MTGL |
| ATOM | 1328 | C | PRO | 171 | 38.497 | -1.472 | 12.039 | 1.00 | 21.36 | MTGL |
| ATOM | 1329 | O | PRO | 171 | 38.790 | -2.009 | 13.109 | 1.00 | 20.24 | MTGL |
| ATOM | 1330 | N | LYS | 172 | 38.351 | -0.161 | 11.908 | 1.00 | 20.37 | MTGL |
| ATOM | 1331 | CA | LYS | 172 | 38.525 | 0.749 | 13.032 | 1.00 | 21.42 | MTGL |
| ATOM | 1332 | CB | LYS | 172 | 38.670 | 2.183 | 12.501 | 1.00 | 22.43 | MTGL |
| ATOM | 1333 | CG | LYS | 172 | 39.602 | 3.071 | 13.310 | 1.00 | 25.68 | MTGL |

# Fig. 1 cont.

| ATOM | 1334 | CD | LYS | 172 | 41.052 | 2.616 | 13.220 | 1.00 | 24.85 | MTGL |
|------|------|------|-----|-----|--------|-------|--------|------|-------|------|
| ATOM | 1335 | CE | LYS | 172 | 41.659 | 2.946 | 11.878 | 1.00 | 25.80 | MTGL |
| ATOM | 1336 | NZ | LYS | 172 | 42.984 | 2.294 | 11.703 | 1.00 | 24.26 | MTGL |
| ATOM | 1337 | C | LYS | 172 | 37.295 | 0.626 | 13.940 | 1.00 | 20.16 | MTGL |
| ATOM | 1338 | O | LYS | 172 | 36.199 | 0.307 | 13.478 | 1.00 | 19.92 | MTGL |
| ATOM | 1339 | N | PRO | 173 | 37.465 | 0.848 | 15.248 | 1.00 | 19.30 | MTGL |
| ATOM | 1340 | CD | PRO | 173 | 38.722 | 1.088 | 15.980 | 1.00 | 19.67 | MTGL |
| ATOM | 1341 | CA | PRO | 173 | 36.335 | 0.751 | 16.177 | 1.00 | 19.05 | MTGL |
| ATOM | 1342 | CB | PRO | 173 | 37.018 | 0.437 | 17.497 | 1.00 | 19.14 | MTGL |
| ATOM | 1343 | CG | PRO | 173 | 38.237 | 1.321 | 17.412 | 1.00 | 18.48 | MTGL |
| ATOM | 1344 | C | PRO | 173 | 35.565 | 2.066 | 16.270 | 1.00 | 18.59 | MTGL |
| ATOM | 1345 | O | PRO | 173 | 36.049 | 3.110 | 15.832 | 1.00 | 16.92 | MTGL |
| ATOM | 1346 | N | LYS | 174 | 34.359 | 2.007 | 16.824 | 1.00 | 17.93 | MTGL |
| ATOM | 1347 | CA | LYS | 174 | 33.591 | 3.222 | 17.037 | 1.00 | 18.70 | MTGL |
| ATOM | 1348 | CB | LYS | 174 | 32.109 | 2.901 | 17.240 | 1.00 | 18.25 | MTGL |
| ATOM | 1349 | CG | LYS | 174 | 31.388 | 2.529 | 15.947 | 1.00 | 19.90 | MTGL |
| ATOM | 1350 | CD | LYS | 174 | 29.937 | 2.142 | 16.200 | 1.00 | 20.92 | MTGL |
| ATOM | 1351 | CE | LYS | 174 | 29.230 | 1.784 | 14.892 | 1.00 | 21.51 | MTGL |
| ATOM | 1352 | NZ | LYS | 174 | 27.839 | 1.317 | 15.135 | 1.00 | 20.89 | MTGL |
| ATOM | 1353 | C | LYS | 174 | 34.193 | 3.808 | 18.318 | 1.00 | 18.48 | MTGL |
| ATOM | 1354 | O | LYS | 174 | 34.452 | 3.076 | 19.281 | 1.00 | 18.00 | MTGL |
| ATOM | 1355 | N | ILE | 175 | 34.448 | 5.112 | 18.320 | 1.00 | 17.76 | MTGL |
| ATOM | 1356 | CA | ILE | 175 | 35.033 | 5.768 | 19.487 | 1.00 | 17.60 | MTGL |
| ATOM | 1357 | CB | ILE | 175 | 35.999 | 6.883 | 19.050 | 1.00 | 17.54 | MTGL |
| ATOM | 1358 | CG2 | ILE | 175 | 36.564 | 7.610 | 20.271 | 1.00 | 17.48 | MTGL |
| ATOM | 1359 | CG1 | ILE | 175 | 37.134 | 6.266 | 18.226 | 1.00 | 16.88 | MTGL |
| ATOM | 1360 | CD1 | ILE | 175 | 38.083 | 7.263 | 17.618 | 1.00 | 15.96 | MTGL |
| ATOM | 1361 | C | ILE | 175 | 33.945 | 6.330 | 20.393 | 1.00 | 17.11 | MTGL |
| ATOM | 1362 | O | ILE | 175 | 33.102 | 7.122 | 19.962 | 1.00 | 17.92 | MTGL |
| ATOM | 1363 | N | MET | 176 | 33.966 | 5.914 | 21.653 | 1.00 | 16.13 | MTGL |
| ATOM | 1364 | CA | MET | 176 | 32.955 | 6.345 | 22.615 | 1.00 | 16.14 | MTGL |
| ATOM | 1365 | CB | MET | 176 | 32.223 | 5.120 | 23.171 | 1.00 | 16.50 | MTGL |
| ATOM | 1366 | CG | MET | 176 | 31.333 | 5.410 | 24.379 | 1.00 | 16.70 | MTGL |
| ATOM | 1367 | SD | MET | 176 | 30.643 | 3.896 | 25.097 | 1.00 | 19.61 | MTGL |
| ATOM | 1368 | CE | MET | 176 | 29.473 | 3.433 | 23.769 | 1.00 | 15.92 | MTGL |
| ATOM | 1369 | C | MET | 176 | 33.458 | 7.163 | 23.797 | 1.00 | 16.18 | MTGL |
| ATOM | 1370 | O | MET | 176 | 34.562 | 6.946 | 24.299 | 1.00 | 15.62 | MTGL |
| ATOM | 1371 | N | ILE | 177 | 32.628 | 8.109 | 24.227 | 1.00 | 16.05 | MTGL |
| ATOM | 1372 | CA | ILE | 177 | 32.915 | 8.927 | 25.402 | 1.00 | 16.22 | MTGL |
| ATOM | 1373 | CB | ILE | 177 | 32.786 | 10.436 | 25.117 | 1.00 | 15.59 | MTGL |
| ATOM | 1374 | CG2 | ILE | 177 | 32.729 | 11.210 | 26.438 | 1.00 | 16.50 | MTGL |
| ATOM | 1375 | CG1 | ILE | 177 | 33.985 | 10.900 | 24.273 | 1.00 | 16.91 | MTGL |
| ATOM | 1376 | CD1 | ILE | 177 | 33.988 | 12.380 | 23.935 | 1.00 | 17.23 | MTGL |
| ATOM | 1377 | C | ILE | 177 | 31.847 | 8.467 | 26.383 | 1.00 | 15.72 | MTGL |
| ATOM | 1378 | O | ILE | 177 | 30.660 | 8.467 | 26.062 | 1.00 | 16.21 | MTGL |
| ATOM | 1379 | N | HIS | 178 | 32.278 | 8.061 | 27.571 | 1.00 | 16.15 | MTGL |
| ATOM | 1380 | CA | HIS | 178 | 31.376 | 7.518 | 28.581 | 1.00 | 16.02 | MTGL |
| ATOM | 1381 | CB | HIS | 178 | 31.866 | 6.112 | 28.949 | 1.00 | 14.76 | MTGL |
| ATOM | 1382 | CG | HIS | 178 | 31.099 | 5.461 | 30.057 | 1.00 | 14.66 | MTGL |
| ATOM | 1383 | CD2 | HIS | 178 | 29.850 | 5.681 | 30.534 | 1.00 | 13.15 | MTGL |
| ATOM | 1384 | ND1 | HIS | 178 | 31.612 | 4.415 | 30.793 | 1.00 | 13.39 | MTGL |
| ATOM | 1385 | CE1 | HIS | 178 | 30.714 | 4.020 | 31.679 | 1.00 | 14.18 | MTGL |
| ATOM | 1386 | NE2 | HIS | 178 | 29.636 | 4.770 | 31.543 | 1.00 | 13.19 | MTGL |
| ATOM | 1387 | C | HIS | 178 | 31.232 | 8.354 | 29.850 | 1.00 | 16.83 | MTGL |
| ATOM | 1388 | O | HIS | 178 | 32.210 | 8.605 | 30.553 | 1.00 | 16.59 | MTGL |
| ATOM | 1389 | N | LEU | 179 | 29.997 | 8.757 | 30.138 | 1.00 | 17.26 | MTGL |
| ATOM | 1390 | CA | LEU | 179 | 29.670 | 9.539 | 31.329 | 1.00 | 18.11 | MTGL |
| ATOM | 1391 | CB | LEU | 179 | 29.014 | 10.866 | 30.925 | 1.00 | 18.73 | MTGL |

## Fig. 1 cont.

| ATOM | 1392 | CG | LEU | 179 | 29.877 | 12.128 | 30.808 | 1.00 | 20.65 | MTGL |
|------|------|-----|-----|-----|--------|--------|--------|------|-------|------|
| ATOM | 1393 | CD1 | LEU | 179 | 31.265 | 11.812 | 30.272 | 1.00 | 19.45 | MTGL |
| ATOM | 1394 | CD2 | LEU | 179 | 29.150 | 13.130 | 29.923 | 1.00 | 20.83 | MTGL |
| ATOM | 1395 | C | LEU | 179 | 28.693 | 8.732 | 32.186 | 1.00 | 18.96 | MTGL |
| ATOM | 1396 | O | LEU | 179 | 27.947 | 7.899 | 31.668 | 1.00 | 19.30 | MTGL |
| ATOM | 1397 | N | ASP | 180 | 28.693 | 8.974 | 33.493 | 1.00 | 18.24 | MTGL |
| ATOM | 1398 | CA | ASP | 180 | 27.780 | 8.267 | 34.385 | 1.00 | 18.02 | MTGL |
| ATOM | 1399 | CB | ASP | 180 | 28.377 | 8.171 | 35.795 | 1.00 | 17.69 | MTGL |
| ATOM | 1400 | CG | ASP | 180 | 28.398 | 9.505 | 36.518 | 1.00 | 19.25 | MTGL |
| ATOM | 1401 | OD1 | ASP | 180 | 28.702 | 10.538 | 35.884 | 1.00 | 19.57 | MTGL |
| ATOM | 1402 | OD2 | ASP | 180 | 28.117 | 9.512 | 37.734 | 1.00 | 20.92 | MTGL |
| ATOM | 1403 | C | ASP | 180 | 26.453 | 9.020 | 34.430 | 1.00 | 18.13 | MTGL |
| ATOM | 1404 | O | ASP | 180 | 26.268 | 9.995 | 33.708 | 1.00 | 17.92 | MTGL |
| ATOM | 1405 | N | ASN | 181 | 25.533 | 8.546 | 35.266 | 1.00 | 19.02 | MTGL |
| ATOM | 1406 | CA | ASN | 181 | 24.219 | 9.165 | 35.439 | 1.00 | 19.13 | MTGL |
| ATOM | 1407 | CB | ASN | 181 | 24.337 | 10.360 | 36.393 | 1.00 | 19.61 | MTGL |
| ATOM | 1408 | CG | ASN | 181 | 24.840 | 9.959 | 37.776 | 1.00 | 20.81 | MTGL |
| ATOM | 1409 | OD1 | ASN | 181 | 24.561 | 8.857 | 38.259 | 1.00 | 20.36 | MTGL |
| ATOM | 1410 | ND2 | ASN | 181 | 25.567 | 10.862 | 38.427 | 1.00 | 21.46 | MTGL |
| ATOM | 1411 | C | ASN | 181 | 23.541 | 9.604 | 34.135 | 1.00 | 19.21 | MTGL |
| ATOM | 1412 | O | ASN | 181 | 23.277 | 10.791 | 33.925 | 1.00 | 18.32 | MTGL |
| ATOM | 1413 | N | GLY | 182 | 23.238 | 8.635 | 33.276 | 1.00 | 18.94 | MTGL |
| ATOM | 1414 | CA | GLY | 182 | 22.610 | 8.937 | 32.003 | 1.00 | 18.55 | MTGL |
| ATOM | 1415 | C | GLY | 182 | 21.309 | 9.704 | 32.101 | 1.00 | 18.91 | MTGL |
| ATOM | 1416 | O | GLY | 182 | 20.952 | 10.428 | 31.179 | 1.00 | 18.95 | MTGL |
| ATOM | 1417 | N | TRP | 183 | 20.609 | 9.546 | 33.219 | 1.00 | 19.65 | MTGL |
| ATOM | 1418 | CA | TRP | 183 | 19.332 | 10.213 | 33.459 | 1.00 | 19.57 | MTGL |
| ATOM | 1419 | CB | TRP | 183 | 18.643 | 9.588 | 34.671 | 1.00 | 20.28 | MTGL |
| ATOM | 1420 | CG | TRP | 183 | 19.515 | 9.586 | 35.904 | 1.00 | 21.43 | MTGL |
| ATOM | 1421 | CD2 | TRP | 183 | 19.671 | 10.653 | 36.856 | 1.00 | 21.48 | MTGL |
| ATOM | 1422 | CE2 | TRP | 183 | 20.614 | 10.222 | 37.816 | 1.00 | 21.25 | MTGL |
| ATOM | 1423 | CE3 | TRP | 183 | 19.103 | 11.931 | 36.989 | 1.00 | 21.53 | MTGL |
| ATOM | 1424 | CD1 | TRP | 183 | 20.348 | 8.585 | 36.316 | 1.00 | 20.88 | MTGL |
| ATOM | 1425 | NE1 | TRP | 183 | 21.011 | 8.959 | 37.463 | 1.00 | 21.48 | MTGL |
| ATOM | 1426 | CZ2 | TRP | 183 | 21.010 | 11.024 | 38.896 | 1.00 | 22.46 | MTGL |
| ATOM | 1427 | CZ3 | TRP | 183 | 19.497 | 12.732 | 38.065 | 1.00 | 21.36 | MTGL |
| ATOM | 1428 | CH2 | TRP | 183 | 20.440 | 12.272 | 39.004 | 1.00 | 21.87 | MTGL |
| ATOM | 1429 | C | TRP | 183 | 19.477 | 11.705 | 33.724 | 1.00 | 20.04 | MTGL |
| ATOM | 1430 | O | TRP | 183 | 18.506 | 12.457 | 33.613 | 1.00 | 19.18 | MTGL |
| ATOM | 1431 | N | ASP | 184 | 20.686 | 12.126 | 34.083 | 1.00 | 20.76 | MTGL |
| ATOM | 1432 | CA | ASP | 184 | 20.957 | 13.522 | 34.417 | 1.00 | 20.14 | MTGL |
| ATOM | 1433 | CB | ASP | 184 | 22.085 | 13.581 | 35.455 | 1.00 | 21.31 | MTGL |
| ATOM | 1434 | CG | ASP | 184 | 22.327 | 14.986 | 35.988 | 1.00 | 24.62 | MTGL |
| ATOM | 1435 | OD1 | ASP | 184 | 21.643 | 15.936 | 35.540 | 1.00 | 24.90 | MTGL |
| ATOM | 1436 | OD2 | ASP | 184 | 23.210 | 15.138 | 36.859 | 1.00 | 25.79 | MTGL |
| ATOM | 1437 | C | ASP | 184 | 21.312 | 14.374 | 33.201 | 1.00 | 20.22 | MTGL |
| ATOM | 1438 | O | ASP | 184 | 22.487 | 14.584 | 32.899 | 1.00 | 19.35 | MTGL |
| ATOM | 1439 | N | TRP | 185 | 20.289 | 14.879 | 32.518 | 1.00 | 19.30 | MTGL |
| ATOM | 1440 | CA | TRP | 185 | 20.498 | 15.704 | 31.333 | 1.00 | 19.09 | MTGL |
| ATOM | 1441 | CB | TRP | 185 | 19.148 | 16.149 | 30.753 | 1.00 | 18.81 | MTGL |
| ATOM | 1442 | CG | TRP | 185 | 19.267 | 17.255 | 29.746 | 1.00 | 18.32 | MTGL |
| ATOM | 1443 | CD2 | TRP | 185 | 20.044 | 17.245 | 28.541 | 1.00 | 18.10 | MTGL |
| ATOM | 1444 | CE2 | TRP | 185 | 19.889 | 18.509 | 27.933 | 1.00 | 18.68 | MTGL |
| ATOM | 1445 | CE3 | TRP | 185 | 20.856 | 16.290 | 27.917 | 1.00 | 18.54 | MTGL |
| ATOM | 1446 | CD1 | TRP | 185 | 18.686 | 18.491 | 29.814 | 1.00 | 18.71 | MTGL |
| ATOM | 1447 | NE1 | TRP | 185 | 19.057 | 19.250 | 28.730 | 1.00 | 18.49 | MTGL |
| ATOM | 1448 | CZ2 | TRP | 185 | 20.518 | 18.845 | 26.732 | 1.00 | 19.18 | MTGL |
| ATOM | 1449 | CZ3 | TRP | 185 | 21.484 | 16.626 | 26.722 | 1.00 | 18.13 | MTGL |

# Fig. 1 cont.

| ATOM | 1450 | CH2 | TRP | 185 | 21.311 | 17.891 | 26.144 | 1.00 | 19.60 | MTGL |
|------|------|-----|-----|-----|--------|--------|--------|------|-------|------|
| ATOM | 1451 | C   | TRP | 185 | 21.360 | 16.931 | 31.626 | 1.00 | 18.76 | MTGL |
| ATOM | 1452 | O   | TRP | 185 | 22.271 | 17.256 | 30.866 | 1.00 | 17.61 | MTGL |
| ATOM | 1453 | N   | GLY | 186 | 21.068 | 17.612 | 32.731 | 1.00 | 19.33 | MTGL |
| ATOM | 1454 | CA  | GLY | 186 | 21.834 | 18.797 | 33.081 | 1.00 | 19.04 | MTGL |
| ATOM | 1455 | C   | GLY | 186 | 23.336 | 18.565 | 33.066 | 1.00 | 19.17 | MTGL |
| ATOM | 1456 | O   | GLY | 186 | 24.098 | 19.353 | 32.505 | 1.00 | 19.02 | MTGL |
| ATOM | 1457 | N   | THR | 187 | 23.772 | 17.473 | 33.677 | 1.00 | 19.36 | MTGL |
| ATOM | 1458 | CA  | THR | 187 | 25.192 | 17.172 | 33.718 | 1.00 | 20.31 | MTGL |
| ATOM | 1459 | CB  | THR | 187 | 25.482 | 16.098 | 34.773 | 1.00 | 21.41 | MTGL |
| ATOM | 1460 | OG1 | THR | 187 | 25.114 | 16.609 | 36.059 | 1.00 | 21.37 | MTGL |
| ATOM | 1461 | CG2 | THR | 187 | 26.964 | 15.735 | 34.781 | 1.00 | 23.08 | MTGL |
| ATOM | 1462 | C   | THR | 187 | 25.731 | 16.745 | 32.359 | 1.00 | 19.27 | MTGL |
| ATOM | 1463 | O   | THR | 187 | 26.815 | 17.166 | 31.965 | 1.00 | 19.21 | MTGL |
| ATOM | 1464 | N   | GLN | 188 | 24.980 | 15.916 | 31.637 | 1.00 | 19.95 | MTGL |
| ATOM | 1465 | CA  | GLN | 188 | 25.420 | 15.479 | 30.312 | 1.00 | 19.24 | MTGL |
| ATOM | 1466 | CB  | GLN | 188 | 24.356 | 14.602 | 29.638 | 1.00 | 19.13 | MTGL |
| ATOM | 1467 | CG  | GLN | 188 | 24.033 | 13.278 | 30.329 | 1.00 | 18.75 | MTGL |
| ATOM | 1468 | CD  | GLN | 188 | 25.203 | 12.299 | 30.339 | 1.00 | 18.38 | MTGL |
| ATOM | 1469 | OE1 | GLN | 188 | 25.874 | 12.099 | 29.328 | 1.00 | 18.47 | MTGL |
| ATOM | 1470 | NE2 | GLN | 188 | 25.435 | 11.675 | 31.483 | 1.00 | 16.34 | MTGL |
| ATOM | 1471 | C   | GLN | 188 | 25.655 | 16.714 | 29.437 | 1.00 | 19.43 | MTGL |
| ATOM | 1472 | O   | GLN | 188 | 26.695 | 16.850 | 28.792 | 1.00 | 18.38 | MTGL |
| ATOM | 1473 | N   | ASN | 189 | 24.673 | 17.612 | 29.429 | 1.00 | 20.01 | MTGL |
| ATOM | 1474 | CA  | ASN | 189 | 24.733 | 18.830 | 28.625 | 1.00 | 20.84 | MTGL |
| ATOM | 1475 | CB  | ASN | 189 | 23.392 | 19.568 | 28.722 | 1.00 | 22.61 | MTGL |
| ATOM | 1476 | CG  | ASN | 189 | 23.323 | 20.781 | 27.813 | 1.00 | 24.36 | MTGL |
| ATOM | 1477 | OD1 | ASN | 189 | 23.788 | 20.744 | 26.674 | 1.00 | 24.74 | MTGL |
| ATOM | 1478 | ND2 | ASN | 189 | 22.725 | 21.860 | 28.310 | 1.00 | 24.46 | MTGL |
| ATOM | 1479 | C   | ASN | 189 | 25.878 | 19.746 | 29.050 | 1.00 | 21.20 | MTGL |
| ATOM | 1480 | O   | ASN | 189 | 26.622 | 20.267 | 28.214 | 1.00 | 20.76 | MTGL |
| ATOM | 1481 | N   | TRP | 190 | 26.015 | 19.935 | 30.356 | 1.00 | 21.74 | MTGL |
| ATOM | 1482 | CA  | TRP | 190 | 27.073 | 20.770 | 30.917 | 1.00 | 22.16 | MTGL |
| ATOM | 1483 | CB  | TRP | 190 | 26.959 | 20.758 | 32.442 | 1.00 | 23.20 | MTGL |
| ATOM | 1484 | CG  | TRP | 190 | 28.143 | 21.315 | 33.192 | 1.00 | 25.19 | MTGL |
| ATOM | 1485 | CD2 | TRP | 190 | 29.121 | 20.563 | 33.925 | 1.00 | 25.40 | MTGL |
| ATOM | 1486 | CE2 | TRP | 190 | 30.015 | 21.491 | 34.505 | 1.00 | 25.48 | MTGL |
| ATOM | 1487 | CE3 | TRP | 190 | 29.336 | 19.194 | 34.137 | 1.00 | 25.81 | MTGL |
| ATOM | 1488 | CD1 | TRP | 190 | 28.474 | 22.632 | 33.355 | 1.00 | 24.81 | MTGL |
| ATOM | 1489 | NE1 | TRP | 190 | 29.595 | 22.744 | 34.146 | 1.00 | 26.35 | MTGL |
| ATOM | 1490 | CZ2 | TRP | 190 | 31.098 | 21.095 | 35.298 | 1.00 | 26.43 | MTGL |
| ATOM | 1491 | CZ3 | TRP | 190 | 30.420 | 18.800 | 34.925 | 1.00 | 26.45 | MTGL |
| ATOM | 1492 | CH2 | TRP | 190 | 31.288 | 19.750 | 35.490 | 1.00 | 25.29 | MTGL |
| ATOM | 1493 | C   | TRP | 190 | 28.451 | 20.252 | 30.493 | 1.00 | 21.86 | MTGL |
| ATOM | 1494 | O   | TRP | 190 | 29.322 | 21.023 | 30.081 | 1.00 | 21.57 | MTGL |
| ATOM | 1495 | N   | TRP | 191 | 28.637 | 18.939 | 30.586 | 1.00 | 20.42 | MTGL |
| ATOM | 1496 | CA  | TRP | 191 | 29.915 | 18.325 | 30.245 | 1.00 | 19.96 | MTGL |
| ATOM | 1497 | CB  | TRP | 191 | 29.902 | 16.846 | 30.631 | 1.00 | 18.89 | MTGL |
| ATOM | 1498 | CG  | TRP | 191 | 31.272 | 16.231 | 30.703 | 1.00 | 18.14 | MTGL |
| ATOM | 1499 | CD2 | TRP | 191 | 32.017 | 15.658 | 29.621 | 1.00 | 17.74 | MTGL |
| ATOM | 1500 | CE2 | TRP | 191 | 33.244 | 15.201 | 30.154 | 1.00 | 17.14 | MTGL |
| ATOM | 1501 | CE3 | TRP | 191 | 31.767 | 15.481 | 28.253 | 1.00 | 17.05 | MTGL |
| ATOM | 1502 | CD1 | TRP | 191 | 32.058 | 16.108 | 31.815 | 1.00 | 18.47 | MTGL |
| ATOM | 1503 | NE1 | TRP | 191 | 33.241 | 15.489 | 31.494 | 1.00 | 16.67 | MTGL |
| ATOM | 1504 | CZ2 | TRP | 191 | 34.221 | 14.583 | 29.366 | 1.00 | 16.52 | MTGL |
| ATOM | 1505 | CZ3 | TRP | 191 | 32.739 | 14.862 | 27.468 | 1.00 | 15.97 | MTGL |
| ATOM | 1506 | CH2 | TRP | 191 | 33.950 | 14.420 | 28.030 | 1.00 | 16.29 | MTGL |
| ATOM | 1507 | C   | TRP | 191 | 30.293 | 18.455 | 28.770 | 1.00 | 19.44 | MTGL |

Fig. 1 cont.

| ATOM | 1508 | O | TRP | 191 | 31.342 | 19.019 | 28.436 | 1.00 | 18.48 | MTGL |
|------|------|-----|-----|-----|--------|--------|--------|------|-------|------|
| ATOM | 1509 | N | TYR | 192 | 29.447 | 17.921 | 27.893 | 1.00 | 19.02 | MTGL |
| ATOM | 1510 | CA | TYR | 192 | 29.707 | 17.961 | 26.455 | 1.00 | 18.88 | MTGL |
| ATOM | 1511 | CB | TYR | 192 | 28.629 | 17.174 | 25.702 | 1.00 | 18.06 | MTGL |
| ATOM | 1512 | CG | TYR | 192 | 28.820 | 15.670 | 25.779 | 1.00 | 17.74 | MTGL |
| ATOM | 1513 | CD1 | TYR | 192 | 29.890 | 15.048 | 25.126 | 1.00 | 17.96 | MTGL |
| ATOM | 1514 | CE1 | TYR | 192 | 30.069 | 13.671 | 25.189 | 1.00 | 18.35 | MTGL |
| ATOM | 1515 | CD2 | TYR | 192 | 27.935 | 14.870 | 26.502 | 1.00 | 16.89 | MTGL |
| ATOM | 1516 | CE2 | TYR | 192 | 28.107 | 13.487 | 26.574 | 1.00 | 17.96 | MTGL |
| ATOM | 1517 | CZ | TYR | 192 | 29.172 | 12.895 | 25.917 | 1.00 | 18.14 | MTGL |
| ATOM | 1518 | OH | TYR | 192 | 29.340 | 11.530 | 25.986 | 1.00 | 19.50 | MTGL |
| ATOM | 1519 | C | TYR | 192 | 29.810 | 19.378 | 25.895 | 1.00 | 19.64 | MTGL |
| ATOM | 1520 | O | TYR | 192 | 30.661 | 19.651 | 25.047 | 1.00 | 17.67 | MTGL |
| ATOM | 1521 | N | THR | 193 | 28.956 | 20.280 | 26.373 | 1.00 | 20.13 | MTGL |
| ATOM | 1522 | CA | THR | 193 | 28.988 | 21.658 | 25.904 | 1.00 | 21.63 | MTGL |
| ATOM | 1523 | CB | THR | 193 | 27.884 | 22.504 | 26.569 | 1.00 | 21.95 | MTGL |
| ATOM | 1524 | OG1 | THR | 193 | 26.600 | 21.990 | 26.195 | 1.00 | 23.39 | MTGL |
| ATOM | 1525 | CG2 | THR | 193 | 27.978 | 23.956 | 26.114 | 1.00 | 23.15 | MTGL |
| ATOM | 1526 | C | THR | 193 | 30.346 | 22.306 | 26.189 | 1.00 | 21.54 | MTGL |
| ATOM | 1527 | O | THR | 193 | 30.978 | 22.863 | 25.291 | 1.00 | 21.18 | MTGL |
| ATOM | 1528 | N | ASN | 194 | 30.804 | 22.218 | 27.434 | 1.00 | 21.85 | MTGL |
| ATOM | 1529 | CA | ASN | 194 | 32.084 | 22.816 | 27.800 | 1.00 | 22.13 | MTGL |
| ATOM | 1530 | CB | ASN | 194 | 32.243 | 22.833 | 29.318 | 1.00 | 23.00 | MTGL |
| ATOM | 1531 | CG | ASN | 194 | 31.437 | 23.944 | 29.968 | 1.00 | 24.26 | MTGL |
| ATOM | 1532 | OD1 | ASN | 194 | 31.675 | 25.123 | 29.709 | 1.00 | 25.08 | MTGL |
| ATOM | 1533 | ND2 | ASN | 194 | 30.478 | 23.573 | 30.810 | 1.00 | 23.61 | MTGL |
| ATOM | 1534 | C | ASN | 194 | 33.292 | 22.146 | 27.156 | 1.00 | 21.45 | MTGL |
| ATOM | 1535 | O | ASN | 194 | 34.266 | 22.813 | 26.815 | 1.00 | 21.18 | MTGL |
| ATOM | 1536 | N | VAL | 195 | 33.236 | 20.831 | 26.986 | 1.00 | 21.36 | MTGL |
| ATOM | 1537 | CA | VAL | 195 | 34.346 | 20.123 | 26.362 | 1.00 | 20.65 | MTGL |
| ATOM | 1538 | CB | VAL | 195 | 34.187 | 18.590 | 26.503 | 1.00 | 20.76 | MTGL |
| ATOM | 1539 | CG1 | VAL | 195 | 35.165 | 17.871 | 25.583 | 1.00 | 19.43 | MTGL |
| ATOM | 1540 | CG2 | VAL | 195 | 34.429 | 18.179 | 27.947 | 1.00 | 20.62 | MTGL |
| ATOM | 1541 | C | VAL | 195 | 34.453 | 20.475 | 24.879 | 1.00 | 21.44 | MTGL |
| ATOM | 1542 | O | VAL | 195 | 35.540 | 20.792 | 24.385 | 1.00 | 20.78 | MTGL |
| ATOM | 1543 | N | LEU | 196 | 33.323 | 20.429 | 24.178 | 1.00 | 21.29 | MTGL |
| ATOM | 1544 | CA | LEU | 196 | 33.300 | 20.712 | 22.746 | 1.00 | 23.23 | MTGL |
| ATOM | 1545 | CB | LEU | 196 | 31.953 | 20.285 | 22.150 | 1.00 | 22.71 | MTGL |
| ATOM | 1546 | CG | LEU | 196 | 31.703 | 18.772 | 22.118 | 1.00 | 24.14 | MTGL |
| ATOM | 1547 | CD1 | LEU | 196 | 30.276 | 18.477 | 21.657 | 1.00 | 22.72 | MTGL |
| ATOM | 1548 | CD2 | LEU | 196 | 32.720 | 18.115 | 21.187 | 1.00 | 23.15 | MTGL |
| ATOM | 1549 | C | LEU | 196 | 33.589 | 22.158 | 22.354 | 1.00 | 24.05 | MTGL |
| ATOM | 1550 | O | LEU | 196 | 34.054 | 22.413 | 21.250 | 1.00 | 24.38 | MTGL |
| ATOM | 1551 | N | LYS | 197 | 33.326 | 23.104 | 23.248 | 1.00 | 25.84 | MTGL |
| ATOM | 1552 | CA | LYS | 197 | 33.562 | 24.506 | 22.919 | 1.00 | 27.64 | MTGL |
| ATOM | 1553 | CB | LYS | 197 | 32.753 | 25.413 | 23.850 | 1.00 | 29.58 | MTGL |
| ATOM | 1554 | CG | LYS | 197 | 33.282 | 25.505 | 25.268 | 1.00 | 32.86 | MTGL |
| ATOM | 1555 | CD | LYS | 197 | 32.239 | 26.101 | 26.207 | 1.00 | 35.16 | MTGL |
| ATOM | 1556 | CE | LYS | 197 | 31.742 | 27.456 | 25.726 | 1.00 | 37.48 | MTGL |
| ATOM | 1557 | NZ | LYS | 197 | 30.672 | 28.001 | 26.617 | 1.00 | 39.55 | MTGL |
| ATOM | 1558 | C | LYS | 197 | 35.038 | 24.897 | 22.956 | 1.00 | 27.59 | MTGL |
| ATOM | 1559 | O | LYS | 197 | 35.397 | 26.010 | 22.577 | 1.00 | 27.09 | MTGL |
| ATOM | 1560 | N | GLN | 198 | 35.896 | 23.980 | 23.395 | 1.00 | 27.10 | MTGL |
| ATOM | 1561 | CA | GLN | 198 | 37.323 | 24.271 | 23.459 | 1.00 | 26.85 | MTGL |
| ATOM | 1562 | CB | GLN | 198 | 38.053 | 23.202 | 24.274 | 1.00 | 26.22 | MTGL |
| ATOM | 1563 | CG | GLN | 198 | 37.608 | 23.127 | 25.718 | 1.00 | 24.93 | MTGL |
| ATOM | 1564 | CD | GLN | 198 | 37.637 | 24.480 | 26.400 | 1.00 | 25.72 | MTGL |
| ATOM | 1565 | OE1 | GLN | 198 | 38.667 | 25.152 | 26.432 | 1.00 | 25.49 | MTGL |

Fig. 1 cont.

| ATOM | 1566 | NE2 | GLN | 198 | 36.501 | 24.886 | 26.950 | 1.00 | 24.69 | MTGL |
|------|------|-----|-----|-----|--------|--------|--------|------|-------|------|
| ATOM | 1567 | C | GLN | 198 | 37.953 | 24.381 | 22.071 | 1.00 | 27.46 | MTGL |
| ATOM | 1568 | O | GLN | 198 | 38.937 | 25.097 | 21.885 | 1.00 | 27.60 | MTGL |
| ATOM | 1569 | N | GLY | 199 | 37.401 | 23.664 | 21.101 | 1.00 | 27.40 | MTGL |
| ATOM | 1570 | CA | GLY | 199 | 37.941 | 23.738 | 19.757 | 1.00 | 28.72 | MTGL |
| ATOM | 1571 | C | GLY | 199 | 39.002 | 22.713 | 19.397 | 1.00 | 29.03 | MTGL |
| ATOM | 1572 | O | GLY | 199 | 39.487 | 22.711 | 18.269 | 1.00 | 30.82 | MTGL |
| ATOM | 1573 | N | THR | 200 | 39.382 | 21.852 | 20.337 | 1.00 | 27.35 | MTGL |
| ATOM | 1574 | CA | THR | 200 | 40.377 | 20.823 | 20.041 | 1.00 | 26.65 | MTGL |
| ATOM | 1575 | CB | THR | 200 | 41.335 | 20.596 | 21.230 | 1.00 | 26.55 | MTGL |
| ATOM | 1576 | OG1 | THR | 200 | 40.579 | 20.447 | 22.438 | 1.00 | 27.05 | MTGL |
| ATOM | 1577 | CG2 | THR | 200 | 42.297 | 21.780 | 21.366 | 1.00 | 26.96 | MTGL |
| ATOM | 1578 | C | THR | 200 | 39.633 | 19.532 | 19.705 | 1.00 | 25.68 | MTGL |
| ATOM | 1579 | O | THR | 200 | 39.665 | 19.072 | 18.569 | 1.00 | 25.00 | MTGL |
| ATOM | 1580 | N | LEU | 201 | 38.960 | 18.947 | 20.690 | 1.00 | 25.02 | MTGL |
| ATOM | 1581 | CA | LEU | 201 | 38.180 | 17.745 | 20.428 | 1.00 | 24.16 | MTGL |
| ATOM | 1582 | CB | LEU | 201 | 37.701 | 17.105 | 21.734 | 1.00 | 23.23 | MTGL |
| ATOM | 1583 | CG | LEU | 201 | 36.814 | 15.867 | 21.556 | 1.00 | 23.41 | MTGL |
| ATOM | 1584 | CD1 | LEU | 201 | 37.674 | 14.680 | 21.136 | 1.00 | 22.70 | MTGL |
| ATOM | 1585 | CD2 | LEU | 201 | 36.099 | 15.552 | 22.852 | 1.00 | 23.70 | MTGL |
| ATOM | 1586 | C | LEU | 201 | 36.967 | 18.221 | 19.628 | 1.00 | 23.81 | MTGL |
| ATOM | 1587 | O | LEU | 201 | 36.280 | 19.152 | 20.041 | 1.00 | 22.98 | MTGL |
| ATOM | 1588 | N | GLU | 202 | 36.710 | 17.608 | 18.480 | 1.00 | 23.89 | MTGL |
| ATOM | 1589 | CA | GLU | 202 | 35.554 | 18.002 | 17.672 | 1.00 | 25.20 | MTGL |
| ATOM | 1590 | CB | GLU | 202 | 35.962 | 18.281 | 16.227 | 1.00 | 26.99 | MTGL |
| ATOM | 1591 | CG | GLU | 202 | 37.142 | 19.208 | 16.054 | 1.00 | 30.89 | MTGL |
| ATOM | 1592 | CD | GLU | 202 | 37.380 | 19.539 | 14.596 | 1.00 | 33.28 | MTGL |
| ATOM | 1593 | OE1 | GLU | 202 | 36.601 | 20.338 | 14.034 | 1.00 | 35.02 | MTGL |
| ATOM | 1594 | OE2 | GLU | 202 | 38.333 | 18.989 | 14.004 | 1.00 | 34.29 | MTGL |
| ATOM | 1595 | C | GLU | 202 | 34.545 | 16.863 | 17.667 | 1.00 | 24.61 | MTGL |
| ATOM | 1596 | O | GLU | 202 | 34.886 | 15.725 | 17.990 | 1.00 | 23.46 | MTGL |
| ATOM | 1597 | N | LEU | 203 | 33.311 | 17.169 | 17.286 | 1.00 | 24.45 | MTGL |
| ATOM | 1598 | CA | LEU | 203 | 32.267 | 16.157 | 17.222 | 1.00 | 25.47 | MTGL |
| ATOM | 1599 | CB | LEU | 203 | 30.959 | 16.768 | 16.721 | 1.00 | 26.23 | MTGL |
| ATOM | 1600 | CG | LEU | 203 | 30.009 | 17.289 | 17.794 | 1.00 | 27.61 | MTGL |
| ATOM | 1601 | CD1 | LEU | 203 | 28.830 | 17.970 | 17.126 | 1.00 | 28.79 | MTGL |
| ATOM | 1602 | CD2 | LEU | 203 | 29.532 | 16.139 | 18.672 | 1.00 | 27.38 | MTGL |
| ATOM | 1603 | C | LEU | 203 | 32.666 | 15.007 | 16.305 | 1.00 | 25.18 | MTGL |
| ATOM | 1604 | O | LEU | 203 | 32.307 | 13.857 | 16.555 | 1.00 | 25.60 | MTGL |
| ATOM | 1605 | N | SER | 204 | 33.411 | 15.318 | 15.249 | 1.00 | 23.52 | MTGL |
| ATOM | 1606 | CA | SER | 204 | 33.841 | 14.295 | 14.305 | 1.00 | 23.46 | MTGL |
| ATOM | 1607 | CB | SER | 204 | 34.367 | 14.941 | 13.016 | 1.00 | 24.47 | MTGL |
| ATOM | 1608 | OG | SER | 204 | 35.559 | 15.677 | 13.253 | 1.00 | 23.17 | MTGL |
| ATOM | 1609 | C | SER | 204 | 34.918 | 13.379 | 14.877 | 1.00 | 22.84 | MTGL |
| ATOM | 1610 | O | SER | 204 | 35.235 | 12.353 | 14.278 | 1.00 | 22.80 | MTGL |
| ATOM | 1611 | N | ASP | 205 | 35.482 | 13.742 | 16.027 | 1.00 | 21.73 | MTGL |
| ATOM | 1612 | CA | ASP | 205 | 36.529 | 12.920 | 16.626 | 1.00 | 21.47 | MTGL |
| ATOM | 1613 | CB | ASP | 205 | 37.369 | 13.735 | 17.616 | 1.00 | 21.78 | MTGL |
| ATOM | 1614 | CG | ASP | 205 | 38.284 | 14.737 | 16.925 | 1.00 | 23.69 | MTGL |
| ATOM | 1615 | OD1 | ASP | 205 | 38.859 | 14.388 | 15.870 | 1.00 | 23.46 | MTGL |
| ATOM | 1616 | OD2 | ASP | 205 | 38.442 | 15.866 | 17.446 | 1.00 | 23.01 | MTGL |
| ATOM | 1617 | C | ASP | 205 | 36.020 | 11.653 | 17.310 | 1.00 | 20.42 | MTGL |
| ATOM | 1618 | O | ASP | 205 | 36.795 | 10.727 | 17.545 | 1.00 | 20.47 | MTGL |
| ATOM | 1619 | N | PHE | 206 | 34.736 | 11.609 | 17.650 | 1.00 | 19.52 | MTGL |
| ATOM | 1620 | CA | PHE | 206 | 34.183 | 10.408 | 18.275 | 1.00 | 20.33 | MTGL |
| ATOM | 1621 | CB | PHE | 206 | 34.060 | 10.565 | 19.801 | 1.00 | 18.69 | MTGL |
| ATOM | 1622 | CG | PHE | 206 | 33.098 | 11.626 | 20.244 | 1.00 | 18.95 | MTGL |
| ATOM | 1623 | CD1 | PHE | 206 | 33.403 | 12.974 | 20.083 | 1.00 | 18.40 | MTGL |

Fig. 1 cont.

| ATOM | 1624 | CD2 | PHE | 206 | 31.899 | 11.275 | 20.861 | 1.00 | 18.16 | MTGL |
|------|------|-----|-----|-----|--------|--------|--------|------|-------|------|
| ATOM | 1625 | CE1 | PHE | 206 | 32.529 | 13.959 | 20.534 | 1.00 | 19.01 | MTGL |
| ATOM | 1626 | CE2 | PHE | 206 | 31.015 | 12.253 | 21.316 | 1.00 | 19.53 | MTGL |
| ATOM | 1627 | CZ  | PHE | 206 | 31.331 | 13.601 | 21.153 | 1.00 | 18.89 | MTGL |
| ATOM | 1628 | C   | PHE | 206 | 32.850 | 10.031 | 17.642 | 1.00 | 20.83 | MTGL |
| ATOM | 1629 | O   | PHE | 206 | 32.267 | 10.825 | 16.901 | 1.00 | 20.91 | MTGL |
| ATOM | 1630 | N   | ASP | 207 | 32.365 | 8.827  | 17.937 | 1.00 | 20.94 | MTGL |
| ATOM | 1631 | CA  | ASP | 207 | 31.134 | 8.331  | 17.322 | 1.00 | 21.05 | MTGL |
| ATOM | 1632 | CB  | ASP | 207 | 31.470 | 7.084  | 16.500 | 1.00 | 21.79 | MTGL |
| ATOM | 1633 | CG  | ASP | 207 | 32.766 | 7.235  | 15.730 | 1.00 | 22.83 | MTGL |
| ATOM | 1634 | OD1 | ASP | 207 | 32.811 | 8.093  | 14.826 | 1.00 | 22.13 | MTGL |
| ATOM | 1635 | OD2 | ASP | 207 | 33.739 | 6.506  | 16.036 | 1.00 | 21.38 | MTGL |
| ATOM | 1636 | C   | ASP | 207 | 29.978 | 7.990  | 18.256 | 1.00 | 20.40 | MTGL |
| ATOM | 1637 | O   | ASP | 207 | 28.813 | 8.022  | 17.847 | 1.00 | 20.09 | MTGL |
| ATOM | 1638 | N   | MET | 208 | 30.286 | 7.660  | 19.502 | 1.00 | 19.17 | MTGL |
| ATOM | 1639 | CA  | MET | 208 | 29.236 | 7.281  | 20.431 | 1.00 | 17.84 | MTGL |
| ATOM | 1640 | CB  | MET | 208 | 29.282 | 5.771  | 20.688 | 1.00 | 17.36 | MTGL |
| ATOM | 1641 | CG  | MET | 208 | 29.319 | 4.900  | 19.455 | 1.00 | 17.72 | MTGL |
| ATOM | 1642 | SD  | MET | 208 | 29.434 | 3.141  | 19.906 | 1.00 | 19.72 | MTGL |
| ATOM | 1643 | CE  | MET | 208 | 27.745 | 2.786  | 20.301 | 1.00 | 18.67 | MTGL |
| ATOM | 1644 | C   | MET | 208 | 29.293 | 7.979  | 21.775 | 1.00 | 17.33 | MTGL |
| ATOM | 1645 | O   | MET | 208 | 30.351 | 8.410  | 22.232 | 1.00 | 16.75 | MTGL |
| ATOM | 1646 | N   | MET | 209 | 28.125 | 8.080  | 22.397 | 1.00 | 16.30 | MTGL |
| ATOM | 1647 | CA  | MET | 209 | 27.991 | 8.653  | 23.722 | 1.00 | 17.25 | MTGL |
| ATOM | 1648 | CB  | MET | 209 | 27.037 | 9.852  | 23.730 | 1.00 | 16.86 | MTGL |
| ATOM | 1649 | CG  | MET | 209 | 27.525 | 11.048 | 22.926 | 1.00 | 17.20 | MTGL |
| ATOM | 1650 | SD  | MET | 209 | 26.439 | 12.511 | 23.096 | 1.00 | 15.98 | MTGL |
| ATOM | 1651 | CE  | MET | 209 | 27.636 | 13.808 | 22.762 | 1.00 | 17.32 | MTGL |
| ATOM | 1652 | C   | MET | 209 | 27.405 | 7.529  | 24.557 | 1.00 | 16.92 | MTGL |
| ATOM | 1653 | O   | MET | 209 | 26.311 | 7.033  | 24.273 | 1.00 | 16.52 | MTGL |
| ATOM | 1654 | N   | GLY | 210 | 28.153 | 7.103  | 25.565 | 1.00 | 16.49 | MTGL |
| ATOM | 1655 | CA  | GLY | 210 | 27.675 | 6.038  | 26.423 | 1.00 | 16.81 | MTGL |
| ATOM | 1656 | C   | GLY | 210 | 27.361 | 6.585  | 27.797 | 1.00 | 16.14 | MTGL |
| ATOM | 1657 | O   | GLY | 210 | 27.991 | 7.537  | 28.257 | 1.00 | 15.66 | MTGL |
| ATOM | 1658 | N   | VAL | 211 | 26.370 | 5.998  | 28.450 | 1.00 | 16.46 | MTGL |
| ATOM | 1659 | CA  | VAL | 211 | 25.999 | 6.431  | 29.784 | 1.00 | 15.55 | MTGL |
| ATOM | 1660 | CB  | VAL | 211 | 24.691 | 7.247  | 29.773 | 1.00 | 15.54 | MTGL |
| ATOM | 1661 | CG1 | VAL | 211 | 24.824 | 8.449  | 28.839 | 1.00 | 16.27 | MTGL |
| ATOM | 1662 | CG2 | VAL | 211 | 23.525 | 6.354  | 29.353 | 1.00 | 14.06 | MTGL |
| ATOM | 1663 | C   | VAL | 211 | 25.781 | 5.236  | 30.700 | 1.00 | 16.00 | MTGL |
| ATOM | 1664 | O   | VAL | 211 | 25.418 | 4.148  | 30.243 | 1.00 | 15.69 | MTGL |
| ATOM | 1665 | N   | SER | 212 | 26.013 | 5.445  | 31.991 | 1.00 | 15.22 | MTGL |
| ATOM | 1666 | CA  | SER | 212 | 25.766 | 4.414  | 32.983 | 1.00 | 15.39 | MTGL |
| ATOM | 1667 | CB  | SER | 212 | 26.741 | 4.537  | 34.158 | 1.00 | 15.48 | MTGL |
| ATOM | 1668 | OG  | SER | 212 | 28.083 | 4.327  | 33.748 | 1.00 | 16.02 | MTGL |
| ATOM | 1669 | C   | SER | 212 | 24.346 | 4.707  | 33.469 | 1.00 | 15.93 | MTGL |
| ATOM | 1670 | O   | SER | 212 | 23.922 | 5.863  | 33.498 | 1.00 | 16.20 | MTGL |
| ATOM | 1671 | N   | PHE | 213 | 23.599 | 3.670  | 33.821 | 1.00 | 15.04 | MTGL |
| ATOM | 1672 | CA  | PHE | 213 | 22.248 | 3.866  | 34.323 | 1.00 | 15.18 | MTGL |
| ATOM | 1673 | CB  | PHE | 213 | 21.218 | 3.762  | 33.191 | 1.00 | 14.75 | MTGL |
| ATOM | 1674 | CG  | PHE | 213 | 19.801 | 3.982  | 33.647 | 1.00 | 14.40 | MTGL |
| ATOM | 1675 | CD1 | PHE | 213 | 19.383 | 5.238  | 34.071 | 1.00 | 15.35 | MTGL |
| ATOM | 1676 | CD2 | PHE | 213 | 18.897 | 2.924  | 33.694 | 1.00 | 14.80 | MTGL |
| ATOM | 1677 | CE1 | PHE | 213 | 18.079 | 5.441  | 34.542 | 1.00 | 15.59 | MTGL |
| ATOM | 1678 | CE2 | PHE | 213 | 17.594 | 3.113  | 34.160 | 1.00 | 15.14 | MTGL |
| ATOM | 1679 | CZ  | PHE | 213 | 17.185 | 4.376  | 34.586 | 1.00 | 15.11 | MTGL |
| ATOM | 1680 | C   | PHE | 213 | 21.956 | 2.821  | 35.388 | 1.00 | 16.01 | MTGL |
| ATOM | 1681 | O   | PHE | 213 | 21.757 | 1.646  | 35.078 | 1.00 | 16.44 | MTGL |

# Fig. 1 cont.

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1682 | N | TYR | 214 | 21.954 | 3.258 | 36.644 | 1.00 | 16.44 | MTGL |
| ATOM | 1683 | CA | TYR | 214 | 21.691 | 2.382 | 37.782 | 1.00 | 16.37 | MTGL |
| ATOM | 1684 | CB | TYR | 214 | 22.917 | 2.332 | 38.700 | 1.00 | 16.76 | MTGL |
| ATOM | 1685 | CG | TYR | 214 | 24.097 | 1.562 | 38.131 | 1.00 | 16.18 | MTGL |
| ATOM | 1686 | CD1 | TYR | 214 | 24.114 | 0.168 | 38.139 | 1.00 | 16.62 | MTGL |
| ATOM | 1687 | CE1 | TYR | 214 | 25.201 | -0.544 | 37.637 | 1.00 | 17.99 | MTGL |
| ATOM | 1688 | CD2 | TYR | 214 | 25.199 | 2.228 | 37.599 | 1.00 | 16.40 | MTGL |
| ATOM | 1689 | CE2 | TYR | 214 | 26.295 | 1.524 | 37.093 | 1.00 | 16.27 | MTGL |
| ATOM | 1690 | CZ | TYR | 214 | 26.288 | 0.142 | 37.118 | 1.00 | 16.37 | MTGL |
| ATOM | 1691 | OH | TYR | 214 | 27.375 | -0.556 | 36.648 | 1.00 | 17.15 | MTGL |
| ATOM | 1692 | C | TYR | 214 | 20.479 | 2.904 | 38.554 | 1.00 | 17.45 | MTGL |
| ATOM | 1693 | O | TYR | 214 | 20.246 | 4.111 | 38.632 | 1.00 | 17.08 | MTGL |
| ATOM | 1694 | N | PRO | 215 | 19.691 | 1.997 | 39.140 | 1.00 | 17.07 | MTGL |
| ATOM | 1695 | CD | PRO | 215 | 19.704 | 0.537 | 38.916 | 1.00 | 17.36 | MTGL |
| ATOM | 1696 | CA | PRO | 215 | 18.506 | 2.395 | 39.896 | 1.00 | 17.11 | MTGL |
| ATOM | 1697 | CB | PRO | 215 | 17.547 | 1.247 | 39.619 | 1.00 | 17.64 | MTGL |
| ATOM | 1698 | CG | PRO | 215 | 18.481 | 0.060 | 39.693 | 1.00 | 17.35 | MTGL |
| ATOM | 1699 | C | PRO | 215 | 18.728 | 2.576 | 41.395 | 1.00 | 18.08 | MTGL |
| ATOM | 1700 | O | PRO | 215 | 17.847 | 3.078 | 42.092 | 1.00 | 17.47 | MTGL |
| ATOM | 1701 | N | PHE | 216 | 19.896 | 2.180 | 41.891 | 1.00 | 18.78 | MTGL |
| ATOM | 1702 | CA | PHE | 216 | 20.152 | 2.251 | 43.328 | 1.00 | 19.20 | MTGL |
| ATOM | 1703 | CB | PHE | 216 | 20.530 | 0.851 | 43.836 | 1.00 | 17.80 | MTGL |
| ATOM | 1704 | CG | PHE | 216 | 21.456 | 0.095 | 42.915 | 1.00 | 18.00 | MTGL |
| ATOM | 1705 | CD1 | PHE | 216 | 22.673 | 0.641 | 42.522 | 1.00 | 18.05 | MTGL |
| ATOM | 1706 | CD2 | PHE | 216 | 21.117 | -1.172 | 42.456 | 1.00 | 17.34 | MTGL |
| ATOM | 1707 | CE1 | PHE | 216 | 23.543 | -0.064 | 41.680 | 1.00 | 17.92 | MTGL |
| ATOM | 1708 | CE2 | PHE | 216 | 21.981 | -1.887 | 41.614 | 1.00 | 17.55 | MTGL |
| ATOM | 1709 | CZ | PHE | 216 | 23.194 | -1.331 | 41.228 | 1.00 | 16.80 | MTGL |
| ATOM | 1710 | C | PHE | 216 | 21.145 | 3.276 | 43.872 | 1.00 | 19.84 | MTGL |
| ATOM | 1711 | O | PHE | 216 | 21.726 | 3.068 | 44.940 | 1.00 | 21.57 | MTGL |
| ATOM | 1712 | N | TYR | 217 | 21.346 | 4.379 | 43.161 | 1.00 | 19.60 | MTGL |
| ATOM | 1713 | CA | TYR | 217 | 22.251 | 5.419 | 43.647 | 1.00 | 20.50 | MTGL |
| ATOM | 1714 | CB | TYR | 217 | 23.468 | 5.575 | 42.732 | 1.00 | 20.09 | MTGL |
| ATOM | 1715 | CG | TYR | 217 | 24.398 | 4.382 | 42.724 | 1.00 | 21.44 | MTGL |
| ATOM | 1716 | CD1 | TYR | 217 | 24.956 | 3.895 | 43.909 | 1.00 | 21.17 | MTGL |
| ATOM | 1717 | CE1 | TYR | 217 | 25.815 | 2.797 | 43.902 | 1.00 | 21.86 | MTGL |
| ATOM | 1718 | CD2 | TYR | 217 | 24.721 | 3.739 | 41.529 | 1.00 | 20.83 | MTGL |
| ATOM | 1719 | CE2 | TYR | 217 | 25.577 | 2.642 | 41.511 | 1.00 | 21.46 | MTGL |
| ATOM | 1720 | CZ | TYR | 217 | 26.120 | 2.174 | 42.697 | 1.00 | 21.33 | MTGL |
| ATOM | 1721 | OH | TYR | 217 | 26.960 | 1.087 | 42.672 | 1.00 | 20.10 | MTGL |
| ATOM | 1722 | C | TYR | 217 | 21.520 | 6.752 | 43.727 | 1.00 | 21.29 | MTGL |
| ATOM | 1723 | O | TYR | 217 | 22.127 | 7.778 | 44.026 | 1.00 | 21.40 | MTGL |
| ATOM | 1724 | N | SER | 218 | 20.218 | 6.725 | 43.450 | 1.00 | 21.47 | MTGL |
| ATOM | 1725 | CA | SER | 218 | 19.387 | 7.926 | 43.475 | 1.00 | 22.44 | MTGL |
| ATOM | 1726 | CB | SER | 218 | 20.043 | 9.050 | 42.677 | 1.00 | 23.02 | MTGL |
| ATOM | 1727 | OG | SER | 218 | 19.128 | 10.108 | 42.463 | 1.00 | 23.85 | MTGL |
| ATOM | 1728 | C | SER | 218 | 18.012 | 7.661 | 42.888 | 1.00 | 22.12 | MTGL |
| ATOM | 1729 | O | SER | 218 | 17.888 | 7.058 | 41.821 | 1.00 | 22.86 | MTGL |
| ATOM | 1730 | N | SER | 219 | 16.980 | 8.128 | 43.577 | 1.00 | 21.77 | MTGL |
| ATOM | 1731 | CA | SER | 219 | 15.615 | 7.938 | 43.111 | 1.00 | 22.44 | MTGL |
| ATOM | 1732 | CB | SER | 219 | 14.624 | 8.308 | 44.216 | 1.00 | 22.46 | MTGL |
| ATOM | 1733 | OG | SER | 219 | 14.793 | 9.658 | 44.607 | 1.00 | 22.44 | MTGL |
| ATOM | 1734 | C | SER | 219 | 15.333 | 8.782 | 41.867 | 1.00 | 22.56 | MTGL |
| ATOM | 1735 | O | SER | 219 | 14.282 | 8.646 | 41.247 | 1.00 | 23.34 | MTGL |
| ATOM | 1736 | N | SER | 220 | 16.267 | 9.653 | 41.503 | 1.00 | 22.13 | MTGL |
| ATOM | 1737 | CA | SER | 220 | 16.088 | 10.488 | 40.319 | 1.00 | 22.61 | MTGL |
| ATOM | 1738 | CB | SER | 220 | 17.037 | 11.691 | 40.358 | 1.00 | 23.25 | MTGL |
| ATOM | 1739 | OG | SER | 220 | 16.688 | 12.584 | 41.403 | 1.00 | 25.72 | MTGL |

# Fig. 1 cont.

| ATOM | 1740 | C   | SER | 220 | 16.330 | 9.704  | 39.032 | 1.00 | 22.26 | MTGL |
|------|------|-----|-----|-----|--------|--------|--------|------|-------|------|
| ATOM | 1741 | O   | SER | 220 | 16.025 | 10.187 | 37.942 | 1.00 | 22.75 | MTGL |
| ATOM | 1742 | N   | ALA | 221 | 16.872 | 8.495  | 39.160 | 1.00 | 20.89 | MTGL |
| ATOM | 1743 | CA  | ALA | 221 | 17.164 | 7.667  | 37.996 | 1.00 | 20.44 | MTGL |
| ATOM | 1744 | CB  | ALA | 221 | 18.266 | 6.644  | 38.343 | 1.00 | 19.75 | MTGL |
| ATOM | 1745 | C   | ALA | 221 | 15.933 | 6.949  | 37.439 | 1.00 | 20.80 | MTGL |
| ATOM | 1746 | O   | ALA | 221 | 15.941 | 5.731  | 37.265 | 1.00 | 20.53 | MTGL |
| ATOM | 1747 | N   | THR | 222 | 14.875 | 7.705  | 37.163 | 1.00 | 20.53 | MTGL |
| ATOM | 1748 | CA  | THR | 222 | 13.651 | 7.134  | 36.607 | 1.00 | 20.82 | MTGL |
| ATOM | 1749 | CB  | THR | 222 | 12.464 | 8.120  | 36.690 | 1.00 | 20.95 | MTGL |
| ATOM | 1750 | OG1 | THR | 222 | 12.792 | 9.310  | 35.966 | 1.00 | 21.38 | MTGL |
| ATOM | 1751 | CG2 | THR | 222 | 12.152 | 8.483  | 38.137 | 1.00 | 21.55 | MTGL |
| ATOM | 1752 | C   | THR | 222 | 13.848 | 6.809  | 35.129 | 1.00 | 20.30 | MTGL |
| ATOM | 1753 | O   | THR | 222 | 14.754 | 7.334  | 34.479 | 1.00 | 20.05 | MTGL |
| ATOM | 1754 | N   | LEU | 223 | 12.990 | 5.947  | 34.598 | 1.00 | 20.97 | MTGL |
| ATOM | 1755 | CA  | LEU | 223 | 13.060 | 5.583  | 33.190 | 1.00 | 20.57 | MTGL |
| ATOM | 1756 | CB  | LEU | 223 | 12.116 | 4.412  | 32.894 | 1.00 | 21.05 | MTGL |
| ATOM | 1757 | CG  | LEU | 223 | 12.455 | 3.097  | 33.612 | 1.00 | 22.20 | MTGL |
| ATOM | 1758 | CD1 | LEU | 223 | 11.415 | 2.039  | 33.276 | 1.00 | 22.93 | MTGL |
| ATOM | 1759 | CD2 | LEU | 223 | 13.841 | 2.629  | 33.195 | 1.00 | 21.13 | MTGL |
| ATOM | 1760 | C   | LEU | 223 | 12.674 | 6.800  | 32.346 | 1.00 | 20.76 | MTGL |
| ATOM | 1761 | O   | LEU | 223 | 13.214 | 7.009  | 31.258 | 1.00 | 19.94 | MTGL |
| ATOM | 1762 | N   | SER | 224 | 11.741 | 7.607  | 32.852 | 1.00 | 20.13 | MTGL |
| ATOM | 1763 | CA  | SER | 224 | 11.311 | 8.804  | 32.128 | 1.00 | 20.71 | MTGL |
| ATOM | 1764 | CB  | SER | 224 | 10.096 | 9.448  | 32.812 | 1.00 | 21.29 | MTGL |
| ATOM | 1765 | OG  | SER | 224 | 10.392 | 9.812  | 34.149 | 1.00 | 26.36 | MTGL |
| ATOM | 1766 | C   | SER | 224 | 12.452 | 9.815  | 32.036 | 1.00 | 18.99 | MTGL |
| ATOM | 1767 | O   | SER | 224 | 12.641 | 10.450 | 30.999 | 1.00 | 19.23 | MTGL |
| ATOM | 1768 | N   | ALA | 225 | 13.214 | 9.967  | 33.115 | 1.00 | 18.09 | MTGL |
| ATOM | 1769 | CA  | ALA | 225 | 14.333 | 10.901 | 33.093 | 1.00 | 17.82 | MTGL |
| ATOM | 1770 | CB  | ALA | 225 | 14.928 | 11.057 | 34.492 | 1.00 | 17.28 | MTGL |
| ATOM | 1771 | C   | ALA | 225 | 15.395 | 10.410 | 32.108 | 1.00 | 17.15 | MTGL |
| ATOM | 1772 | O   | ALA | 225 | 16.018 | 11.208 | 31.410 | 1.00 | 18.25 | MTGL |
| ATOM | 1773 | N   | LEU | 226 | 15.598 | 9.097  | 32.048 | 1.00 | 16.97 | MTGL |
| ATOM | 1774 | CA  | LEU | 226 | 16.580 | 8.534  | 31.122 | 1.00 | 17.41 | MTGL |
| ATOM | 1775 | CB  | LEU | 226 | 16.693 | 7.017  | 31.303 | 1.00 | 17.39 | MTGL |
| ATOM | 1776 | CG  | LEU | 226 | 17.711 | 6.325  | 30.389 | 1.00 | 17.54 | MTGL |
| ATOM | 1777 | CD1 | LEU | 226 | 19.109 | 6.852  | 30.679 | 1.00 | 17.23 | MTGL |
| ATOM | 1778 | CD2 | LEU | 226 | 17.658 | 4.824  | 30.606 | 1.00 | 17.56 | MTGL |
| ATOM | 1779 | C   | LEU | 226 | 16.126 | 8.839  | 29.696 | 1.00 | 17.60 | MTGL |
| ATOM | 1780 | O   | LEU | 226 | 16.909 | 9.311  | 28.868 | 1.00 | 17.24 | MTGL |
| ATOM | 1781 | N   | LYS | 227 | 14.854 | 8.566  | 29.423 | 1.00 | 17.18 | MTGL |
| ATOM | 1782 | CA  | LYS | 227 | 14.277 | 8.811  | 28.105 | 1.00 | 18.16 | MTGL |
| ATOM | 1783 | CB  | LYS | 227 | 12.780 | 8.488  | 28.120 | 1.00 | 18.24 | MTGL |
| ATOM | 1784 | CG  | LYS | 227 | 12.007 | 8.984  | 26.890 | 1.00 | 18.81 | MTGL |
| ATOM | 1785 | CD  | LYS | 227 | 12.540 | 8.394  | 25.590 | 1.00 | 17.63 | MTGL |
| ATOM | 1786 | CE  | LYS | 227 | 11.629 | 8.737  | 24.411 | 1.00 | 18.20 | MTGL |
| ATOM | 1787 | NZ  | LYS | 227 | 12.191 | 8.269  | 23.111 | 1.00 | 17.92 | MTGL |
| ATOM | 1788 | C   | LYS | 227 | 14.476 | 10.258 | 27.668 | 1.00 | 18.40 | MTGL |
| ATOM | 1789 | O   | LYS | 227 | 14.978 | 10.526 | 26.576 | 1.00 | 18.56 | MTGL |
| ATOM | 1790 | N   | SER | 228 | 14.078 | 11.190 | 28.529 | 1.00 | 18.71 | MTGL |
| ATOM | 1791 | CA  | SER | 228 | 14.209 | 12.610 | 28.225 | 1.00 | 18.63 | MTGL |
| ATOM | 1792 | CB  | SER | 228 | 13.584 | 13.449 | 29.344 | 1.00 | 19.90 | MTGL |
| ATOM | 1793 | OG  | SER | 228 | 13.763 | 14.835 | 29.096 | 1.00 | 20.80 | MTGL |
| ATOM | 1794 | C   | SER | 228 | 15.662 | 13.022 | 28.024 | 1.00 | 18.30 | MTGL |
| ATOM | 1795 | O   | SER | 228 | 15.973 | 13.778 | 27.106 | 1.00 | 18.71 | MTGL |
| ATOM | 1796 | N   | SER | 229 | 16.553 | 12.525 | 28.880 | 1.00 | 17.99 | MTGL |
| ATOM | 1797 | CA  | SER | 229 | 17.969 | 12.862 | 28.768 | 1.00 | 18.28 | MTGL |

Fig. 1 cont.

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1798 | CB | SER | 229 | 18.752 | 12.299 | 29.962 | 1.00 | 18.83 | MTGL |
| ATOM | 1799 | OG | SER | 229 | 20.127 | 12.641 | 29.867 | 1.00 | 17.92 | MTGL |
| ATOM | 1800 | C | SER | 229 | 18.577 | 12.339 | 27.463 | 1.00 | 18.05 | MTGL |
| ATOM | 1801 | O | SER | 229 | 19.251 | 13.076 | 26.744 | 1.00 | 18.70 | MTGL |
| ATOM | 1802 | N | LEU | 230 | 18.338 | 11.070 | 27.149 | 1.00 | 17.87 | MTGL |
| ATOM | 1803 | CA | LEU | 230 | 18.884 | 10.503 | 25.920 | 1.00 | 17.26 | MTGL |
| ATOM | 1804 | CB | LEU | 230 | 18.620 | 8.994 | 25.860 | 1.00 | 16.24 | MTGL |
| ATOM | 1805 | CG | LEU | 230 | 19.265 | 8.162 | 26.976 | 1.00 | 16.12 | MTGL |
| ATOM | 1806 | CD1 | LEU | 230 | 19.069 | 6.676 | 26.671 | 1.00 | 16.29 | MTGL |
| ATOM | 1807 | CD2 | LEU | 230 | 20.749 | 8.473 | 27.084 | 1.00 | 12.97 | MTGL |
| ATOM | 1808 | C | LEU | 230 | 18.299 | 11.204 | 24.689 | 1.00 | 17.08 | MTGL |
| ATOM | 1809 | O | LEU | 230 | 19.014 | 11.458 | 23.721 | 1.00 | 15.52 | MTGL |
| ATOM | 1810 | N | ASP | 231 | 17.006 | 11.525 | 24.728 | 1.00 | 18.20 | MTGL |
| ATOM | 1811 | CA | ASP | 231 | 16.380 | 12.223 | 23.604 | 1.00 | 18.97 | MTGL |
| ATOM | 1812 | CB | ASP | 231 | 14.896 | 12.494 | 23.878 | 1.00 | 20.35 | MTGL |
| ATOM | 1813 | CG | ASP | 231 | 13.985 | 11.337 | 23.455 | 1.00 | 20.69 | MTGL |
| ATOM | 1814 | OD1 | ASP | 231 | 14.460 | 10.361 | 22.838 | 1.00 | 21.48 | MTGL |
| ATOM | 1815 | OD2 | ASP | 231 | 12.775 | 11.418 | 23.738 | 1.00 | 20.71 | MTGL |
| ATOM | 1816 | C | ASP | 231 | 17.102 | 13.553 | 23.393 | 1.00 | 19.05 | MTGL |
| ATOM | 1817 | O | ASP | 231 | 17.423 | 13.927 | 22.265 | 1.00 | 20.05 | MTGL |
| ATOM | 1818 | N | ASN | 232 | 17.369 | 14.260 | 24.486 | 1.00 | 18.97 | MTGL |
| ATOM | 1819 | CA | ASN | 232 | 18.057 | 15.546 | 24.403 | 1.00 | 19.27 | MTGL |
| ATOM | 1820 | CB | ASN | 232 | 18.126 | 16.219 | 25.781 | 1.00 | 19.34 | MTGL |
| ATOM | 1821 | CG | ASN | 232 | 16.775 | 16.752 | 26.238 | 1.00 | 21.88 | MTGL |
| ATOM | 1822 | OD1 | ASN | 232 | 15.911 | 17.054 | 25.420 | 1.00 | 23.78 | MTGL |
| ATOM | 1823 | ND2 | ASN | 232 | 16.595 | 16.882 | 27.545 | 1.00 | 21.09 | MTGL |
| ATOM | 1824 | C | ASN | 232 | 19.459 | 15.397 | 23.834 | 1.00 | 19.42 | MTGL |
| ATOM | 1825 | O | ASN | 232 | 19.887 | 16.205 | 23.003 | 1.00 | 19.51 | MTGL |
| ATOM | 1826 | N | MET | 233 | 20.174 | 14.368 | 24.280 | 1.00 | 19.18 | MTGL |
| ATOM | 1827 | CA | MET | 233 | 21.533 | 14.124 | 23.803 | 1.00 | 19.15 | MTGL |
| ATOM | 1828 | CB | MET | 233 | 22.151 | 12.936 | 24.551 | 1.00 | 18.27 | MTGL |
| ATOM | 1829 | CG | MET | 233 | 22.433 | 13.191 | 26.029 | 1.00 | 19.33 | MTGL |
| ATOM | 1830 | SD | MET | 233 | 22.806 | 11.662 | 26.940 | 1.00 | 19.17 | MTGL |
| ATOM | 1831 | CE | MET | 233 | 24.330 | 11.165 | 26.125 | 1.00 | 17.20 | MTGL |
| ATOM | 1832 | C | MET | 233 | 21.510 | 13.833 | 22.305 | 1.00 | 19.80 | MTGL |
| ATOM | 1833 | O | MET | 233 | 22.356 | 14.314 | 21.547 | 1.00 | 19.41 | MTGL |
| ATOM | 1834 | N | ALA | 234 | 20.529 | 13.043 | 21.885 | 1.00 | 20.01 | MTGL |
| ATOM | 1835 | CA | ALA | 234 | 20.390 | 12.673 | 20.480 | 1.00 | 21.04 | MTGL |
| ATOM | 1836 | CB | ALA | 234 | 19.274 | 11.633 | 20.324 | 1.00 | 19.66 | MTGL |
| ATOM | 1837 | C | ALA | 234 | 20.111 | 13.879 | 19.583 | 1.00 | 21.48 | MTGL |
| ATOM | 1838 | O | ALA | 234 | 20.761 | 14.055 | 18.549 | 1.00 | 20.87 | MTGL |
| ATOM | 1839 | N | LYS | 235 | 19.156 | 14.715 | 19.985 | 1.00 | 22.48 | MTGL |
| ATOM | 1840 | CA | LYS | 235 | 18.804 | 15.881 | 19.176 | 1.00 | 24.12 | MTGL |
| ATOM | 1841 | CB | LYS | 235 | 17.507 | 16.515 | 19.681 | 1.00 | 26.52 | MTGL |
| ATOM | 1842 | CG | LYS | 235 | 17.053 | 17.695 | 18.835 | 1.00 | 33.00 | MTGL |
| ATOM | 1843 | CD | LYS | 235 | 15.744 | 18.274 | 19.331 | 1.00 | 36.39 | MTGL |
| ATOM | 1844 | CE | LYS | 235 | 15.288 | 19.436 | 18.451 | 1.00 | 40.33 | MTGL |
| ATOM | 1845 | NZ | LYS | 235 | 13.979 | 19.997 | 18.912 | 1.00 | 42.05 | MTGL |
| ATOM | 1846 | C | LYS | 235 | 19.900 | 16.937 | 19.145 | 1.00 | 22.78 | MTGL |
| ATOM | 1847 | O | LYS | 235 | 20.041 | 17.660 | 18.169 | 1.00 | 21.57 | MTGL |
| ATOM | 1848 | N | THR | 236 | 20.688 | 17.014 | 20.209 | 1.00 | 23.01 | MTGL |
| ATOM | 1849 | CA | THR | 236 | 21.753 | 18.004 | 20.280 | 1.00 | 22.42 | MTGL |
| ATOM | 1850 | CB | THR | 236 | 22.146 | 18.289 | 21.744 | 1.00 | 22.63 | MTGL |
| ATOM | 1851 | OG1 | THR | 236 | 20.973 | 18.616 | 22.495 | 1.00 | 23.14 | MTGL |
| ATOM | 1852 | CG2 | THR | 236 | 23.118 | 19.459 | 21.818 | 1.00 | 22.49 | MTGL |
| ATOM | 1853 | C | THR | 236 | 23.020 | 17.635 | 19.506 | 1.00 | 22.72 | MTGL |
| ATOM | 1854 | O | THR | 236 | 23.556 | 18.468 | 18.773 | 1.00 | 22.41 | MTGL |
| ATOM | 1855 | N | TRP | 237 | 23.495 | 16.398 | 19.655 | 1.00 | 21.45 | MTGL |

Fig. 1 cont.

| ATOM | 1856 | CA  | TRP | 237 | 24.728 | 15.984 | 18.984 | 1.00 | 21.17 | MTGL |
|------|------|-----|-----|-----|--------|--------|--------|------|-------|------|
| ATOM | 1857 | CB  | TRP | 237 | 25.773 | 15.621 | 20.041 | 1.00 | 21.53 | MTGL |
| ATOM | 1858 | CG  | TRP | 237 | 26.103 | 16.796 | 20.916 | 1.00 | 21.36 | MTGL |
| ATOM | 1859 | CD2 | TRP | 237 | 25.684 | 17.004 | 22.270 | 1.00 | 20.90 | MTGL |
| ATOM | 1860 | CE2 | TRP | 237 | 26.156 | 18.274 | 22.662 | 1.00 | 20.29 | MTGL |
| ATOM | 1861 | CE3 | TRP | 237 | 24.957 | 16.237 | 23.191 | 1.00 | 20.64 | MTGL |
| ATOM | 1862 | CD1 | TRP | 237 | 26.795 | 17.920 | 20.554 | 1.00 | 21.20 | MTGL |
| ATOM | 1863 | NE1 | TRP | 237 | 26.827 | 18.811 | 21.595 | 1.00 | 19.36 | MTGL |
| ATOM | 1864 | CZ2 | TRP | 237 | 25.919 | 18.799 | 23.935 | 1.00 | 20.39 | MTGL |
| ATOM | 1865 | CZ3 | TRP | 237 | 24.724 | 16.760 | 24.458 | 1.00 | 20.25 | MTGL |
| ATOM | 1866 | CH2 | TRP | 237 | 25.205 | 18.028 | 24.817 | 1.00 | 20.45 | MTGL |
| ATOM | 1867 | C   | TRP | 237 | 24.600 | 14.868 | 17.941 | 1.00 | 21.19 | MTGL |
| ATOM | 1868 | O   | TRP | 237 | 25.561 | 14.555 | 17.238 | 1.00 | 20.33 | MTGL |
| ATOM | 1869 | N   | ASN | 238 | 23.414 | 14.274 | 17.865 | 0.50 | 21.58 | MTGL |
| ATOM | 1870 | CA  | ASN | 238 | 23.119 | 13.212 | 16.908 | 0.50 | 21.97 | MTGL |
| ATOM | 1871 | CB  | ASN | 238 | 22.847 | 13.829 | 15.534 | 0.50 | 23.20 | MTGL |
| ATOM | 1872 | CG  | ASN | 238 | 21.696 | 14.822 | 15.560 | 0.50 | 24.82 | MTGL |
| ATOM | 1873 | OD1 | ASN | 238 | 20.631 | 14.540 | 16.107 | 0.50 | 25.88 | MTGL |
| ATOM | 1874 | ND2 | ASN | 238 | 21.904 | 15.989 | 14.960 | 0.50 | 26.50 | MTGL |
| ATOM | 1875 | C   | ASN | 238 | 24.179 | 12.113 | 16.782 | 0.50 | 21.69 | MTGL |
| ATOM | 1876 | O   | ASN | 238 | 24.564 | 11.730 | 15.678 | 0.50 | 21.51 | MTGL |
| ATOM | 1877 | N   | LYS | 239 | 24.644 | 11.607 | 17.919 | 1.00 | 21.56 | MTGL |
| ATOM | 1878 | CA  | LYS | 239 | 25.639 | 10.534 | 17.938 | 1.00 | 20.81 | MTGL |
| ATOM | 1879 | CB  | LYS | 239 | 26.732 | 10.832 | 18.971 | 1.00 | 21.93 | MTGL |
| ATOM | 1880 | CG  | LYS | 239 | 27.684 | 11.957 | 18.598 | 1.00 | 21.60 | MTGL |
| ATOM | 1881 | CD  | LYS | 239 | 28.521 | 11.569 | 17.396 | 1.00 | 23.06 | MTGL |
| ATOM | 1882 | CE  | LYS | 239 | 29.543 | 12.633 | 17.053 | 1.00 | 23.30 | MTGL |
| ATOM | 1883 | NZ  | LYS | 239 | 30.266 | 12.280 | 15.800 | 1.00 | 22.03 | MTGL |
| ATOM | 1884 | C   | LYS | 239 | 24.927 | 9.243  | 18.331 | 1.00 | 20.23 | MTGL |
| ATOM | 1885 | O   | LYS | 239 | 23.814 | 9.287  | 18.856 | 1.00 | 19.43 | MTGL |
| ATOM | 1886 | N   | GLU | 240 | 25.548 | 8.096  | 18.072 | 1.00 | 19.70 | MTGL |
| ATOM | 1887 | CA  | GLU | 240 | 24.933 | 6.835  | 18.467 | 1.00 | 19.84 | MTGL |
| ATOM | 1888 | CB  | GLU | 240 | 25.702 | 5.633  | 17.912 | 1.00 | 21.53 | MTGL |
| ATOM | 1889 | CG  | GLU | 240 | 25.612 | 5.485  | 16.402 | 1.00 | 24.54 | MTGL |
| ATOM | 1890 | CD  | GLU | 240 | 25.950 | 4.081  | 15.930 | 1.00 | 26.26 | MTGL |
| ATOM | 1891 | OE1 | GLU | 240 | 26.984 | 3.532  | 16.366 | 1.00 | 27.61 | MTGL |
| ATOM | 1892 | OE2 | GLU | 240 | 25.179 | 3.527  | 15.118 | 1.00 | 28.35 | MTGL |
| ATOM | 1893 | C   | GLU | 240 | 24.972 | 6.823  | 19.985 | 1.00 | 18.12 | MTGL |
| ATOM | 1894 | O   | GLU | 240 | 25.945 | 7.269  | 20.589 | 1.00 | 16.94 | MTGL |
| ATOM | 1895 | N   | ILE | 241 | 23.910 | 6.320  | 20.598 | 1.00 | 17.17 | MTGL |
| ATOM | 1896 | CA  | ILE | 241 | 23.816 | 6.290  | 22.049 | 1.00 | 17.75 | MTGL |
| ATOM | 1897 | CB  | ILE | 241 | 22.639 | 7.161  | 22.509 | 1.00 | 18.47 | MTGL |
| ATOM | 1898 | CG2 | ILE | 241 | 22.411 | 6.997  | 24.013 | 1.00 | 19.08 | MTGL |
| ATOM | 1899 | CG1 | ILE | 241 | 22.918 | 8.617  | 22.126 | 1.00 | 17.74 | MTGL |
| ATOM | 1900 | CD1 | ILE | 241 | 21.732 | 9.539  | 22.297 | 1.00 | 18.08 | MTGL |
| ATOM | 1901 | C   | ILE | 241 | 23.651 | 4.894  | 22.625 | 1.00 | 17.68 | MTGL |
| ATOM | 1902 | O   | ILE | 241 | 23.020 | 4.026  | 22.015 | 1.00 | 16.98 | MTGL |
| ATOM | 1903 | N   | ALA | 242 | 24.219 | 4.683  | 23.809 | 1.00 | 17.80 | MTGL |
| ATOM | 1904 | CA  | ALA | 242 | 24.115 | 3.389  | 24.465 | 1.00 | 17.48 | MTGL |
| ATOM | 1905 | CB  | ALA | 242 | 25.170 | 2.433  | 23.906 | 1.00 | 16.79 | MTGL |
| ATOM | 1906 | C   | ALA | 242 | 24.244 | 3.457  | 25.977 | 1.00 | 16.97 | MTGL |
| ATOM | 1907 | O   | ALA | 242 | 24.966 | 4.291  | 26.520 | 1.00 | 16.47 | MTGL |
| ATOM | 1908 | N   | VAL | 243 | 23.505 | 2.586  | 26.654 | 1.00 | 16.88 | MTGL |
| ATOM | 1909 | CA  | VAL | 243 | 23.594 | 2.478  | 28.098 | 1.00 | 16.35 | MTGL |
| ATOM | 1910 | CB  | VAL | 243 | 22.261 | 2.003  | 28.715 | 1.00 | 15.54 | MTGL |
| ATOM | 1911 | CG1 | VAL | 243 | 22.470 | 1.580  | 30.159 | 1.00 | 16.43 | MTGL |
| ATOM | 1912 | CG2 | VAL | 243 | 21.238 | 3.133  | 28.655 | 1.00 | 15.23 | MTGL |
| ATOM | 1913 | C   | VAL | 243 | 24.667 | 1.396  | 28.212 | 1.00 | 16.01 | MTGL |

Fig. 1 cont.

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1914 | O | VAL | 243 | 24.424 | 0.243 | 27.856 | 1.00 | 16.07 | MTGL |
| ATOM | 1915 | N | VAL | 244 | 25.860 | 1.774 | 28.665 | 1.00 | 15.48 | MTGL |
| ATOM | 1916 | CA | VAL | 244 | 26.971 | 0.822 | 28.758 | 1.00 | 15.55 | MTGL |
| ATOM | 1917 | CB | VAL | 244 | 28.292 | 1.501 | 28.345 | 1.00 | 15.25 | MTGL |
| ATOM | 1918 | CG1 | VAL | 244 | 28.167 | 2.024 | 26.922 | 1.00 | 15.71 | MTGL |
| ATOM | 1919 | CG2 | VAL | 244 | 28.618 | 2.646 | 29.294 | 1.00 | 14.98 | MTGL |
| ATOM | 1920 | C | VAL | 244 | 27.163 | 0.125 | 30.097 | 1.00 | 15.27 | MTGL |
| ATOM | 1921 | O | VAL | 244 | 28.052 | -0.710 | 30.244 | 1.00 | 16.53 | MTGL |
| ATOM | 1922 | N | GLU | 245 | 26.326 | 0.464 | 31.068 | 1.00 | 15.31 | MTGL |
| ATOM | 1923 | CA | GLU | 245 | 26.387 | -0.145 | 32.391 | 1.00 | 15.54 | MTGL |
| ATOM | 1924 | CB | GLU | 245 | 27.390 | 0.581 | 33.301 | 1.00 | 15.71 | MTGL |
| ATOM | 1925 | CG | GLU | 245 | 28.833 | 0.193 | 33.105 | 1.00 | 17.89 | MTGL |
| ATOM | 1926 | CD | GLU | 245 | 29.738 | 0.777 | 34.177 | 1.00 | 19.37 | MTGL |
| ATOM | 1927 | OE1 | GLU | 245 | 29.322 | 0.824 | 35.359 | 1.00 | 18.55 | MTGL |
| ATOM | 1928 | OE2 | GLU | 245 | 30.867 | 1.174 | 33.827 | 1.00 | 20.37 | MTGL |
| ATOM | 1929 | C | GLU | 245 | 25.024 | -0.053 | 33.043 | 1.00 | 15.41 | MTGL |
| ATOM | 1930 | O | GLU | 245 | 24.421 | 1.014 | 33.060 | 1.00 | 16.55 | MTGL |
| ATOM | 1931 | N | THR | 246 | 24.533 | -1.174 | 33.563 | 1.00 | 15.11 | MTGL |
| ATOM | 1932 | CA | THR | 246 | 23.266 | -1.185 | 34.280 | 1.00 | 14.75 | MTGL |
| ATOM | 1933 | CB | THR | 246 | 22.053 | -1.052 | 33.322 | 1.00 | 15.60 | MTGL |
| ATOM | 1934 | OG1 | THR | 246 | 20.884 | -0.721 | 34.085 | 1.00 | 14.95 | MTGL |
| ATOM | 1935 | CG2 | THR | 246 | 21.809 | -2.352 | 32.564 | 1.00 | 14.91 | MTGL |
| ATOM | 1936 | C | THR | 246 | 23.168 | -2.467 | 35.100 | 1.00 | 14.67 | MTGL |
| ATOM | 1937 | O | THR | 246 | 23.853 | -3.451 | 34.807 | 1.00 | 15.70 | MTGL |
| ATOM | 1938 | N | ASN | 247 | 22.331 | -2.441 | 36.134 | 1.00 | 14.38 | MTGL |
| ATOM | 1939 | CA | ASN | 247 | 22.128 | -3.579 | 37.035 | 1.00 | 14.91 | MTGL |
| ATOM | 1940 | CB | ASN | 247 | 23.012 | -3.462 | 38.294 | 1.00 | 15.25 | MTGL |
| ATOM | 1941 | CG | ASN | 247 | 24.397 | -4.085 | 38.150 | 1.00 | 16.92 | MTGL |
| ATOM | 1942 | OD1 | ASN | 247 | 25.212 | -3.972 | 39.068 | 1.00 | 16.53 | MTGL |
| ATOM | 1943 | ND2 | ASN | 247 | 24.668 | -4.746 | 37.024 | 1.00 | 14.82 | MTGL |
| ATOM | 1944 | C | ASN | 247 | 20.693 | -3.554 | 37.560 | 1.00 | 15.99 | MTGL |
| ATOM | 1945 | O | ASN | 247 | 20.057 | -2.496 | 37.609 | 1.00 | 15.64 | MTGL |
| ATOM | 1946 | N | TRP | 248 | 20.194 | -4.723 | 37.946 | 1.00 | 15.53 | MTGL |
| ATOM | 1947 | CA | TRP | 248 | 18.893 | -4.830 | 38.600 | 1.00 | 16.36 | MTGL |
| ATOM | 1948 | CB | TRP | 248 | 17.732 | -5.127 | 37.657 | 1.00 | 14.84 | MTGL |
| ATOM | 1949 | CG | TRP | 248 | 16.455 | -5.135 | 38.445 | 1.00 | 13.73 | MTGL |
| ATOM | 1950 | CD2 | TRP | 248 | 15.743 | -3.989 | 38.940 | 1.00 | 14.11 | MTGL |
| ATOM | 1951 | CE2 | TRP | 248 | 14.684 | -4.467 | 39.739 | 1.00 | 12.13 | MTGL |
| ATOM | 1952 | CE3 | TRP | 248 | 15.902 | -2.603 | 38.786 | 1.00 | 14.57 | MTGL |
| ATOM | 1953 | CD1 | TRP | 248 | 15.812 | -6.224 | 38.949 | 1.00 | 13.26 | MTGL |
| ATOM | 1954 | NE1 | TRP | 248 | 14.751 | -5.833 | 39.728 | 1.00 | 13.69 | MTGL |
| ATOM | 1955 | CZ2 | TRP | 248 | 13.784 | -3.613 | 40.384 | 1.00 | 14.00 | MTGL |
| ATOM | 1956 | CZ3 | TRP | 248 | 15.008 | -1.751 | 39.427 | 1.00 | 13.98 | MTGL |
| ATOM | 1957 | CH2 | TRP | 248 | 13.962 | -2.260 | 40.218 | 1.00 | 14.50 | MTGL |
| ATOM | 1958 | C | TRP | 248 | 19.080 | -5.972 | 39.576 | 1.00 | 16.41 | MTGL |
| ATOM | 1959 | O | TRP | 248 | 19.507 | -7.060 | 39.200 | 1.00 | 17.70 | MTGL |
| ATOM | 1960 | N | PRO | 249 | 18.765 | -5.739 | 40.850 | 1.00 | 17.62 | MTGL |
| ATOM | 1961 | CD | PRO | 249 | 18.316 | -4.468 | 41.449 | 1.00 | 17.41 | MTGL |
| ATOM | 1962 | CA | PRO | 249 | 18.933 | -6.774 | 41.868 | 1.00 | 17.81 | MTGL |
| ATOM | 1963 | CB | PRO | 249 | 19.010 | -5.961 | 43.156 | 1.00 | 18.08 | MTGL |
| ATOM | 1964 | CG | PRO | 249 | 18.056 | -4.857 | 42.892 | 1.00 | 20.03 | MTGL |
| ATOM | 1965 | C | PRO | 249 | 17.922 | -7.898 | 41.972 | 1.00 | 18.16 | MTGL |
| ATOM | 1966 | O | PRO | 249 | 16.729 | -7.722 | 41.728 | 1.00 | 18.74 | MTGL |
| ATOM | 1967 | N | ILE | 250 | 18.426 | -9.074 | 42.322 | 1.00 | 18.86 | MTGL |
| ATOM | 1968 | CA | ILE | 250 | 17.561 | -10.215 | 42.549 | 1.00 | 20.06 | MTGL |
| ATOM | 1969 | CB | ILE | 250 | 18.189 | -11.544 | 42.040 | 1.00 | 20.52 | MTGL |
| ATOM | 1970 | CG2 | ILE | 250 | 18.230 | -11.553 | 40.518 | 1.00 | 19.08 | MTGL |
| ATOM | 1971 | CG1 | ILE | 250 | 19.590 | -11.734 | 42.614 | 1.00 | 20.81 | MTGL |

Fig. 1 cont.

| ATOM | 1972 | CD1 | ILE | 250 | 20.222 | -13.061 | 42.216 | 1.00 | 21.09 | MTGL |
|------|------|-----|-----|-----|--------|---------|--------|------|-------|------|
| ATOM | 1973 | C   | ILE | 250 | 17.408 | -10.234 | 44.075 | 1.00 | 19.97 | MTGL |
| ATOM | 1974 | O   | ILE | 250 | 16.659 | -11.028 | 44.637 | 1.00 | 20.48 | MTGL |
| ATOM | 1975 | N   | SER | 251 | 18.127 | -9.327  | 44.735 | 1.00 | 20.21 | MTGL |
| ATOM | 1976 | CA  | SER | 251 | 18.072 | -9.206  | 46.188 | 1.00 | 21.30 | MTGL |
| ATOM | 1977 | CB  | SER | 251 | 18.878 | -10.331 | 46.843 | 1.00 | 22.63 | MTGL |
| ATOM | 1978 | OG  | SER | 251 | 18.757 | -10.273 | 48.253 | 1.00 | 24.04 | MTGL |
| ATOM | 1979 | C   | SER | 251 | 18.603 | -7.855  | 46.658 | 1.00 | 21.50 | MTGL |
| ATOM | 1980 | O   | SER | 251 | 19.735 | -7.485  | 46.343 | 1.00 | 21.25 | MTGL |
| ATOM | 1981 | N   | CYS | 252 | 17.784 | -7.112  | 47.400 | 1.00 | 21.87 | MTGL |
| ATOM | 1982 | CA  | CYS | 252 | 18.194 | -5.806  | 47.918 | 1.00 | 23.27 | MTGL |
| ATOM | 1983 | C   | CYS | 252 | 17.529 | -5.505  | 49.263 | 1.00 | 24.17 | MTGL |
| ATOM | 1984 | O   | CYS | 252 | 16.654 | -4.647  | 49.340 | 1.00 | 24.61 | MTGL |
| ATOM | 1985 | CB  | CYS | 252 | 17.840 | -4.684  | 46.927 | 1.00 | 23.57 | MTGL |
| ATOM | 1986 | SG  | CYS | 252 | 18.756 | -3.154  | 47.311 | 1.00 | 23.83 | MTGL |
| ATOM | 1987 | N   | PRO | 253 | 17.951 | -6.199  | 50.340 | 1.00 | 25.34 | MTGL |
| ATOM | 1988 | CD  | PRO | 253 | 18.950 | -7.281  | 50.290 | 1.00 | 26.08 | MTGL |
| ATOM | 1989 | CA  | PRO | 253 | 17.428 | -6.052  | 51.707 | 1.00 | 25.93 | MTGL |
| ATOM | 1990 | CB  | PRO | 253 | 18.308 | -7.001  | 52.518 | 1.00 | 26.63 | MTGL |
| ATOM | 1991 | CG  | PRO | 253 | 18.627 | -8.068  | 51.539 | 1.00 | 27.12 | MTGL |
| ATOM | 1992 | C   | PRO | 253 | 17.416 | -4.645  | 52.294 | 1.00 | 26.16 | MTGL |
| ATOM | 1993 | O   | PRO | 253 | 16.415 | -4.223  | 52.865 | 1.00 | 26.46 | MTGL |
| ATOM | 1994 | N   | ASN | 254 | 18.526 | -3.922  | 52.178 | 1.00 | 26.96 | MTGL |
| ATOM | 1995 | CA  | ASN | 254 | 18.574 | -2.560  | 52.713 | 1.00 | 27.76 | MTGL |
| ATOM | 1996 | CB  | ASN | 254 | 19.145 | -2.538  | 54.137 | 1.00 | 29.54 | MTGL |
| ATOM | 1997 | CG  | ASN | 254 | 20.541 | -3.097  | 54.220 | 1.00 | 31.33 | MTGL |
| ATOM | 1998 | OD1 | ASN | 254 | 20.854 | -4.102  | 53.587 | 1.00 | 34.28 | MTGL |
| ATOM | 1999 | ND2 | ASN | 254 | 21.388 | -2.465  | 55.028 | 1.00 | 30.87 | MTGL |
| ATOM | 2000 | C   | ASN | 254 | 19.329 | -1.580  | 51.834 | 1.00 | 26.98 | MTGL |
| ATOM | 2001 | O   | ASN | 254 | 20.525 | -1.355  | 51.990 | 1.00 | 26.72 | MTGL |
| ATOM | 2002 | N   | PRO | 255 | 18.623 | -0.993  | 50.873 | 1.00 | 26.12 | MTGL |
| ATOM | 2003 | CD  | PRO | 255 | 17.274 | -1.385  | 50.443 | 1.00 | 25.65 | MTGL |
| ATOM | 2004 | CA  | PRO | 255 | 19.222 | -0.023  | 49.957 | 1.00 | 25.15 | MTGL |
| ATOM | 2005 | CB  | PRO | 255 | 18.128 | 0.211   | 48.913 | 1.00 | 25.50 | MTGL |
| ATOM | 2006 | CG  | PRO | 255 | 16.895 | -0.262  | 49.550 | 1.00 | 25.88 | MTGL |
| ATOM | 2007 | C   | PRO | 255 | 19.638 | 1.279   | 50.637 | 1.00 | 25.08 | MTGL |
| ATOM | 2008 | O   | PRO | 255 | 18.993 | 1.735   | 51.586 | 1.00 | 24.66 | MTGL |
| ATOM | 2009 | N   | ARG | 256 | 20.717 | 1.869   | 50.128 | 1.00 | 23.54 | MTGL |
| ATOM | 2010 | CA  | ARG | 256 | 21.219 | 3.131   | 50.653 | 1.00 | 24.56 | MTGL |
| ATOM | 2011 | CB  | ARG | 256 | 22.679 | 3.345   | 50.230 | 1.00 | 26.20 | MTGL |
| ATOM | 2012 | CG  | ARG | 256 | 23.290 | 4.673   | 50.685 | 1.00 | 29.88 | MTGL |
| ATOM | 2013 | CD  | ARG | 256 | 23.244 | 4.843   | 52.205 | 1.00 | 33.75 | MTGL |
| ATOM | 2014 | NE  | ARG | 256 | 24.112 | 3.900   | 52.913 | 1.00 | 36.98 | MTGL |
| ATOM | 2015 | CZ  | ARG | 256 | 24.215 | 3.826   | 54.241 | 1.00 | 38.13 | MTGL |
| ATOM | 2016 | NH1 | ARG | 256 | 23.503 | 4.683   | 55.016 | 1.00 | 37.96 | MTGL |
| ATOM | 2017 | NH2 | ARG | 256 | 25.034 | 2.942   | 54.796 | 1.00 | 38.27 | MTGL |
| ATOM | 2018 | C   | ARG | 256 | 20.346 | 4.291   | 50.152 | 1.00 | 24.09 | MTGL |
| ATOM | 2019 | O   | ARG | 256 | 20.223 | 5.312   | 50.820 | 1.00 | 22.82 | MTGL |
| ATOM | 2020 | N   | TYR | 257 | 19.740 | 4.129   | 48.978 | 1.00 | 23.76 | MTGL |
| ATOM | 2021 | CA  | TYR | 257 | 18.869 | 5.162   | 48.417 | 1.00 | 24.47 | MTGL |
| ATOM | 2022 | CB  | TYR | 257 | 19.506 | 5.829   | 47.197 | 1.00 | 25.66 | MTGL |
| ATOM | 2023 | CG  | TYR | 257 | 20.889 | 6.365   | 47.430 | 1.00 | 27.18 | MTGL |
| ATOM | 2024 | CD1 | TYR | 257 | 22.003 | 5.538   | 47.316 | 1.00 | 27.30 | MTGL |
| ATOM | 2025 | CE1 | TYR | 257 | 23.283 | 6.020   | 47.567 | 1.00 | 28.24 | MTGL |
| ATOM | 2026 | CD2 | TYR | 257 | 21.086 | 7.693   | 47.802 | 1.00 | 28.37 | MTGL |
| ATOM | 2027 | CE2 | TYR | 257 | 22.363 | 8.184   | 48.058 | 1.00 | 28.50 | MTGL |
| ATOM | 2028 | CZ  | TYR | 257 | 23.455 | 7.341   | 47.940 | 1.00 | 29.46 | MTGL |
| ATOM | 2029 | OH  | TYR | 257 | 24.720 | 7.814   | 48.215 | 1.00 | 30.61 | MTGL |

Fig. 1 cont.

| ATOM | 2030 | C   | TYR | 257 | 17.539 | 4.578  | 47.986 | 1.00 | 24.30 | MTGL |
|------|------|-----|-----|-----|--------|--------|--------|------|-------|------|
| ATOM | 2031 | O   | TYR | 257 | 17.450 | 3.408  | 47.619 | 1.00 | 24.04 | MTGL |
| ATOM | 2032 | N   | SER | 258 | 16.507 | 5.411  | 48.018 | 1.00 | 24.57 | MTGL |
| ATOM | 2033 | CA  | SER | 258 | 15.178 | 4.984  | 47.607 | 1.00 | 24.95 | MTGL |
| ATOM | 2034 | CB  | SER | 258 | 14.162 | 6.084  | 47.930 | 1.00 | 25.55 | MTGL |
| ATOM | 2035 | OG  | SER | 258 | 14.261 | 6.471  | 49.292 | 1.00 | 27.69 | MTGL |
| ATOM | 2036 | C   | SER | 258 | 15.230 | 4.746  | 46.102 | 1.00 | 23.31 | MTGL |
| ATOM | 2037 | O   | SER | 258 | 15.949 | 5.449  | 45.392 | 1.00 | 23.48 | MTGL |
| ATOM | 2038 | N   | PHE | 259 | 14.488 | 3.754  | 45.619 | 1.00 | 22.69 | MTGL |
| ATOM | 2039 | CA  | PHE | 259 | 14.459 | 3.452  | 44.190 | 1.00 | 23.46 | MTGL |
| ATOM | 2040 | CB  | PHE | 259 | 13.961 | 2.022  | 43.958 | 1.00 | 22.78 | MTGL |
| ATOM | 2041 | CG  | PHE | 259 | 15.051 | 0.990  | 43.984 | 1.00 | 22.99 | MTGL |
| ATOM | 2042 | CD1 | PHE | 259 | 15.923 | 0.904  | 45.066 | 1.00 | 24.03 | MTGL |
| ATOM | 2043 | CD2 | PHE | 259 | 15.218 | 0.112  | 42.919 | 1.00 | 22.03 | MTGL |
| ATOM | 2044 | CE1 | PHE | 259 | 16.945 | -0.046 | 45.089 | 1.00 | 24.16 | MTGL |
| ATOM | 2045 | CE2 | PHE | 259 | 16.233 | -0.839 | 42.929 | 1.00 | 22.81 | MTGL |
| ATOM | 2046 | CZ  | PHE | 259 | 17.103 | -0.918 | 44.019 | 1.00 | 23.26 | MTGL |
| ATOM | 2047 | C   | PHE | 259 | 13.580 | 4.429  | 43.411 | 1.00 | 23.33 | MTGL |
| ATOM | 2048 | O   | PHE | 259 | 12.681 | 5.048  | 43.975 | 1.00 | 23.29 | MTGL |
| ATOM | 2049 | N   | PRO | 260 | 13.840 | 4.581  | 42.100 | 1.00 | 23.87 | MTGL |
| ATOM | 2050 | CD  | PRO | 260 | 14.959 | 4.002  | 41.338 | 1.00 | 23.34 | MTGL |
| ATOM | 2051 | CA  | PRO | 260 | 13.057 | 5.492  | 41.259 | 1.00 | 23.83 | MTGL |
| ATOM | 2052 | CB  | PRO | 260 | 13.711 | 5.346  | 39.888 | 1.00 | 23.96 | MTGL |
| ATOM | 2053 | CG  | PRO | 260 | 15.138 | 5.012  | 40.229 | 1.00 | 23.75 | MTGL |
| ATOM | 2054 | C   | PRO | 260 | 11.594 | 5.062  | 41.255 | 1.00 | 24.68 | MTGL |
| ATOM | 2055 | O   | PRO | 260 | 11.287 | 3.867  | 41.233 | 1.00 | 22.71 | MTGL |
| ATOM | 2056 | N   | SER | 261 | 10.700 | 6.042  | 41.274 | 1.00 | 24.81 | MTGL |
| ATOM | 2057 | CA  | SER | 261 | 9.267  | 5.783  | 41.298 | 1.00 | 25.73 | MTGL |
| ATOM | 2058 | CB  | SER | 261 | 8.494  | 7.107  | 41.254 | 1.00 | 26.69 | MTGL |
| ATOM | 2059 | OG  | SER | 261 | 8.667  | 7.757  | 40.003 | 1.00 | 27.65 | MTGL |
| ATOM | 2060 | C   | SER | 261 | 8.725  | 4.862  | 40.207 | 1.00 | 25.31 | MTGL |
| ATOM | 2061 | O   | SER | 261 | 7.853  | 4.048  | 40.488 | 1.00 | 25.28 | MTGL |
| ATOM | 2062 | N   | ASP | 262 | 9.214  | 4.979  | 38.973 | 1.00 | 26.49 | MTGL |
| ATOM | 2063 | CA  | ASP | 262 | 8.678  | 4.131  | 37.909 | 1.00 | 27.78 | MTGL |
| ATOM | 2064 | CB  | ASP | 262 | 8.762  | 4.824  | 36.535 | 1.00 | 27.44 | MTGL |
| ATOM | 2065 | CG  | ASP | 262 | 10.166 | 5.267  | 36.170 | 1.00 | 29.75 | MTGL |
| ATOM | 2066 | OD1 | ASP | 262 | 11.138 | 4.673  | 36.681 | 1.00 | 29.62 | MTGL |
| ATOM | 2067 | OD2 | ASP | 262 | 10.289 | 6.207  | 35.349 | 1.00 | 29.82 | MTGL |
| ATOM | 2068 | C   | ASP | 262 | 9.259  | 2.724  | 37.816 | 1.00 | 28.89 | MTGL |
| ATOM | 2069 | O   | ASP | 262 | 9.063  | 2.037  | 36.812 | 1.00 | 29.03 | MTGL |
| ATOM | 2070 | N   | VAL | 263 | 9.968  | 2.291  | 38.857 | 1.00 | 29.21 | MTGL |
| ATOM | 2071 | CA  | VAL | 263 | 10.529 | 0.941  | 38.878 | 1.00 | 29.98 | MTGL |
| ATOM | 2072 | CB  | VAL | 263 | 12.063 | 0.930  | 38.613 | 1.00 | 29.51 | MTGL |
| ATOM | 2073 | CG1 | VAL | 263 | 12.355 | 1.468  | 37.226 | 1.00 | 28.86 | MTGL |
| ATOM | 2074 | CG2 | VAL | 263 | 12.788 | 1.751  | 39.669 | 1.00 | 29.09 | MTGL |
| ATOM | 2075 | C   | VAL | 263 | 10.254 | 0.257  | 40.218 | 1.00 | 30.76 | MTGL |
| ATOM | 2076 | O   | VAL | 263 | 10.672 | -0.879 | 40.434 | 1.00 | 30.49 | MTGL |
| ATOM | 2077 | N   | LYS | 264 | 9.534  | 0.941  | 41.108 | 1.00 | 31.82 | MTGL |
| ATOM | 2078 | CA  | LYS | 264 | 9.215  | 0.394  | 42.432 | 1.00 | 33.07 | MTGL |
| ATOM | 2079 | CB  | LYS | 264 | 8.570  | 1.464  | 43.317 | 1.00 | 34.40 | MTGL |
| ATOM | 2080 | CG  | LYS | 264 | 9.566  | 2.391  | 44.002 | 1.00 | 36.45 | MTGL |
| ATOM | 2081 | CD  | LYS | 264 | 8.859  | 3.344  | 44.961 | 1.00 | 38.24 | MTGL |
| ATOM | 2082 | CE  | LYS | 264 | 9.844  | 4.281  | 45.655 | 1.00 | 40.37 | MTGL |
| ATOM | 2083 | NZ  | LYS | 264 | 9.148  | 5.291  | 46.508 | 1.00 | 40.59 | MTGL |
| ATOM | 2084 | C   | LYS | 264 | 8.321  | -0.842 | 42.415 | 1.00 | 33.40 | MTGL |
| ATOM | 2085 | O   | LYS | 264 | 8.267  | -1.595 | 43.394 | 1.00 | 33.28 | MTGL |
| ATOM | 2086 | N   | ASN | 265 | 7.612  | -1.049 | 41.313 | 1.00 | 32.77 | MTGL |
| ATOM | 2087 | CA  | ASN | 265 | 6.738  | -2.208 | 41.194 | 1.00 | 32.23 | MTGL |

Fig. 1 cont.

| ATOM | 2088 | CB  | ASN | 265 | 5.587  | -1.898  | 40.236 | 1.00 | 34.35 | MTGL |
|------|------|-----|-----|-----|--------|---------|--------|------|-------|------|
| ATOM | 2089 | CG  | ASN | 265 | 6.074  | -1.544  | 38.845 | 1.00 | 36.81 | MTGL |
| ATOM | 2090 | OD1 | ASN | 265 | 6.837  | -0.593  | 38.667 | 1.00 | 37.33 | MTGL |
| ATOM | 2091 | ND2 | ASN | 265 | 5.638  | -2.311  | 37.848 | 1.00 | 38.71 | MTGL |
| ATOM | 2092 | C   | ASN | 265 | 7.504  | -3.436  | 40.689 | 1.00 | 30.70 | MTGL |
| ATOM | 2093 | O   | ASN | 265 | 6.998  | -4.555  | 40.744 | 1.00 | 30.83 | MTGL |
| ATOM | 2094 | N   | ILE | 266 | 8.719  | -3.226  | 40.192 | 1.00 | 28.28 | MTGL |
| ATOM | 2095 | CA  | ILE | 266 | 9.517  | -4.336  | 39.687 | 1.00 | 25.48 | MTGL |
| ATOM | 2096 | CB  | ILE | 266 | 10.651 | -3.848  | 38.767 | 1.00 | 23.96 | MTGL |
| ATOM | 2097 | CG2 | ILE | 266 | 11.449 | -5.046  | 38.257 | 1.00 | 23.40 | MTGL |
| ATOM | 2098 | CG1 | ILE | 266 | 10.067 | -3.054  | 37.594 | 1.00 | 23.38 | MTGL |
| ATOM | 2099 | CD1 | ILE | 266 | 11.114 | -2.516  | 36.627 | 1.00 | 22.30 | MTGL |
| ATOM | 2100 | C   | ILE | 266 | 10.122 | -5.094  | 40.867 | 1.00 | 24.88 | MTGL |
| ATOM | 2101 | O   | ILE | 266 | 10.825 | -4.520  | 41.691 | 1.00 | 22.68 | MTGL |
| ATOM | 2102 | N   | PRO | 267 | 9.850  | -6.404  | 40.960 | 1.00 | 24.25 | MTGL |
| ATOM | 2103 | CD  | PRO | 267 | 9.012  | -7.212  | 40.051 | 1.00 | 23.79 | MTGL |
| ATOM | 2104 | CA  | PRO | 267 | 10.374 | -7.225  | 42.052 | 1.00 | 23.72 | MTGL |
| ATOM | 2105 | CB  | PRO | 267 | 9.542  | -8.497  | 41.946 | 1.00 | 24.48 | MTGL |
| ATOM | 2106 | CG  | PRO | 267 | 9.373  | -8.633  | 40.455 | 1.00 | 24.22 | MTGL |
| ATOM | 2107 | C   | PRO | 267 | 11.865 | -7.526  | 41.943 | 1.00 | 23.20 | MTGL |
| ATOM | 2108 | O   | PRO | 267 | 12.437 | -7.515  | 40.851 | 1.00 | 22.29 | MTGL |
| ATOM | 2109 | N   | PHE | 268 | 12.487 | -7.781  | 43.090 | 1.00 | 22.29 | MTGL |
| ATOM | 2110 | CA  | PHE | 268 | 13.898 | -8.134  | 43.119 | 1.00 | 22.67 | MTGL |
| ATOM | 2111 | CB  | PHE | 268 | 14.533 | -7.757  | 44.462 | 1.00 | 22.68 | MTGL |
| ATOM | 2112 | CG  | PHE | 268 | 14.493 | -6.285  | 44.754 | 1.00 | 22.93 | MTGL |
| ATOM | 2113 | CD1 | PHE | 268 | 14.838 | -5.360  | 43.773 | 1.00 | 22.68 | MTGL |
| ATOM | 2114 | CD2 | PHE | 268 | 14.115 | -5.821  | 46.008 | 1.00 | 23.18 | MTGL |
| ATOM | 2115 | CE1 | PHE | 268 | 14.806 | -3.993  | 44.037 | 1.00 | 23.40 | MTGL |
| ATOM | 2116 | CE2 | PHE | 268 | 14.079 | -4.454  | 46.283 | 1.00 | 23.36 | MTGL |
| ATOM | 2117 | CZ  | PHE | 268 | 14.425 | -3.539  | 45.298 | 1.00 | 23.35 | MTGL |
| ATOM | 2118 | C   | PHE | 268 | 13.925 | -9.643  | 42.921 | 1.00 | 21.88 | MTGL |
| ATOM | 2119 | O   | PHE | 268 | 13.780 | -10.414 | 43.873 | 1.00 | 21.02 | MTGL |
| ATOM | 2120 | N   | SER | 269 | 14.088 | -10.049 | 41.667 | 1.00 | 21.08 | MTGL |
| ATOM | 2121 | CA  | SER | 269 | 14.110 | -11.457 | 41.294 | 1.00 | 20.72 | MTGL |
| ATOM | 2122 | CB  | SER | 269 | 12.702 | -12.052 | 41.417 | 1.00 | 19.79 | MTGL |
| ATOM | 2123 | OG  | SER | 269 | 11.814 | -11.416 | 40.509 | 1.00 | 19.06 | MTGL |
| ATOM | 2124 | C   | SER | 269 | 14.554 | -11.546 | 39.844 | 1.00 | 20.32 | MTGL |
| ATOM | 2125 | O   | SER | 269 | 14.670 | -10.530 | 39.161 | 1.00 | 19.97 | MTGL |
| ATOM | 2126 | N   | PRO | 270 | 14.814 | -12.767 | 39.354 | 1.00 | 21.15 | MTGL |
| ATOM | 2127 | CD  | PRO | 270 | 14.896 | -14.054 | 40.075 | 1.00 | 20.43 | MTGL |
| ATOM | 2128 | CA  | PRO | 270 | 15.237 | -12.915 | 37.958 | 1.00 | 20.91 | MTGL |
| ATOM | 2129 | CB  | PRO | 270 | 15.407 | -14.426 | 37.809 | 1.00 | 20.78 | MTGL |
| ATOM | 2130 | CG  | PRO | 270 | 15.832 | -14.852 | 39.196 | 1.00 | 20.58 | MTGL |
| ATOM | 2131 | C   | PRO | 270 | 14.169 | -12.348 | 37.016 | 1.00 | 20.97 | MTGL |
| ATOM | 2132 | O   | PRO | 270 | 14.489 | -11.688 | 36.028 | 1.00 | 20.64 | MTGL |
| ATOM | 2133 | N   | GLU | 271 | 12.900 | -12.605 | 37.331 | 1.00 | 21.15 | MTGL |
| ATOM | 2134 | CA  | GLU | 271 | 11.797 | -12.102 | 36.508 | 1.00 | 21.55 | MTGL |
| ATOM | 2135 | CB  | GLU | 271 | 10.446 | -12.538 | 37.082 | 1.00 | 22.38 | MTGL |
| ATOM | 2136 | CG  | GLU | 271 | 10.155 | -14.036 | 37.003 | 1.00 | 25.49 | MTGL |
| ATOM | 2137 | CD  | GLU | 271 | 11.082 | -14.873 | 37.870 | 1.00 | 26.37 | MTGL |
| ATOM | 2138 | OE1 | GLU | 271 | 11.447 | -14.415 | 38.970 | 1.00 | 26.39 | MTGL |
| ATOM | 2139 | OE2 | GLU | 271 | 11.433 | -15.997 | 37.457 | 1.00 | 27.82 | MTGL |
| ATOM | 2140 | C   | GLU | 271 | 11.861 | -10.577 | 36.476 | 1.00 | 20.84 | MTGL |
| ATOM | 2141 | O   | GLU | 271 | 11.640 | -9.949  | 35.434 | 1.00 | 20.80 | MTGL |
| ATOM | 2142 | N   | GLY | 272 | 12.166 | -9.993  | 37.631 | 1.00 | 19.71 | MTGL |
| ATOM | 2143 | CA  | GLY | 272 | 12.271 | -8.550  | 37.734 | 1.00 | 18.93 | MTGL |
| ATOM | 2144 | C   | GLY | 272 | 13.415 | -8.008  | 36.897 | 1.00 | 18.95 | MTGL |
| ATOM | 2145 | O   | GLY | 272 | 13.284 | -6.941  | 36.289 | 1.00 | 19.13 | MTGL |

# Fig. 1 cont.

| ATOM | 2146 | N   | GLN | 273 | 14.534 | -8.734  | 36.859 | 1.00 | 17.61 | MTGL |
| ATOM | 2147 | CA  | GLN | 273 | 15.687 | -8.299  | 36.074 | 1.00 | 18.43 | MTGL |
| ATOM | 2148 | CB  | GLN | 273 | 16.864 | -9.260  | 36.230 | 1.00 | 17.76 | MTGL |
| ATOM | 2149 | CG  | GLN | 273 | 17.467 | -9.345  | 37.610 | 1.00 | 19.26 | MTGL |
| ATOM | 2150 | CD  | GLN | 273 | 18.720 | -10.190 | 37.607 | 1.00 | 19.87 | MTGL |
| ATOM | 2151 | OE1 | GLN | 273 | 18.726 | -11.304 | 37.073 | 1.00 | 18.60 | MTGL |
| ATOM | 2152 | NE2 | GLN | 273 | 19.793 | -9.667  | 38.198 | 1.00 | 19.12 | MTGL |
| ATOM | 2153 | C   | GLN | 273 | 15.300 | -8.270  | 34.607 | 1.00 | 18.09 | MTGL |
| ATOM | 2154 | O   | GLN | 273 | 15.660 | -7.353  | 33.869 | 1.00 | 17.98 | MTGL |
| ATOM | 2155 | N   | THR | 274 | 14.579 | -9.305  | 34.193 | 1.00 | 17.84 | MTGL |
| ATOM | 2156 | CA  | THR | 274 | 14.131 | -9.433  | 32.815 | 1.00 | 17.91 | MTGL |
| ATOM | 2157 | CB  | THR | 274 | 13.293 | -10.712 | 32.637 | 1.00 | 18.13 | MTGL |
| ATOM | 2158 | OG1 | THR | 274 | 14.128 | -11.857 | 32.859 | 1.00 | 19.81 | MTGL |
| ATOM | 2159 | CG2 | THR | 274 | 12.695 | -10.777 | 31.231 | 1.00 | 19.04 | MTGL |
| ATOM | 2160 | C   | THR | 274 | 13.293 | -8.219  | 32.428 | 1.00 | 17.34 | MTGL |
| ATOM | 2161 | O   | THR | 274 | 13.504 | -7.619  | 31.376 | 1.00 | 16.72 | MTGL |
| ATOM | 2162 | N   | THR | 275 | 12.351 | -7.859  | 33.294 | 1.00 | 16.98 | MTGL |
| ATOM | 2163 | CA  | THR | 275 | 11.483 | -6.712  | 33.056 | 1.00 | 17.24 | MTGL |
| ATOM | 2164 | CB  | THR | 275 | 10.425 | -6.574  | 34.169 | 1.00 | 17.29 | MTGL |
| ATOM | 2165 | OG1 | THR | 275 | 9.587  | -7.735  | 34.181 | 1.00 | 17.49 | MTGL |
| ATOM | 2166 | CG2 | THR | 275 | 9.563  | -5.331  | 33.937 | 1.00 | 16.88 | MTGL |
| ATOM | 2167 | C   | THR | 275 | 12.270 | -5.405  | 32.982 | 1.00 | 17.05 | MTGL |
| ATOM | 2168 | O   | THR | 275 | 12.090 | -4.618  | 32.052 | 1.00 | 17.86 | MTGL |
| ATOM | 2169 | N   | PHE | 276 | 13.139 | -5.174  | 33.963 | 1.00 | 16.71 | MTGL |
| ATOM | 2170 | CA  | PHE | 276 | 13.937 | -3.949  | 34.000 | 1.00 | 15.62 | MTGL |
| ATOM | 2171 | CB  | PHE | 276 | 14.781 | -3.890  | 35.278 | 1.00 | 15.45 | MTGL |
| ATOM | 2172 | CG  | PHE | 276 | 15.621 | -2.646  | 35.389 | 1.00 | 16.62 | MTGL |
| ATOM | 2173 | CD1 | PHE | 276 | 15.048 | -1.437  | 35.777 | 1.00 | 17.56 | MTGL |
| ATOM | 2174 | CD2 | PHE | 276 | 16.976 | -2.675  | 35.077 | 1.00 | 17.00 | MTGL |
| ATOM | 2175 | CE1 | PHE | 276 | 15.817 | -0.272  | 35.860 | 1.00 | 18.40 | MTGL |
| ATOM | 2176 | CE2 | PHE | 276 | 17.757 | -1.518  | 35.155 | 1.00 | 18.28 | MTGL |
| ATOM | 2177 | CZ  | PHE | 276 | 17.176 | -0.314  | 35.546 | 1.00 | 17.73 | MTGL |
| ATOM | 2178 | C   | PHE | 276 | 14.866 | -3.825  | 32.796 | 1.00 | 16.42 | MTGL |
| ATOM | 2179 | O   | PHE | 276 | 14.907 | -2.785  | 32.136 | 1.00 | 17.18 | MTGL |
| ATOM | 2180 | N   | ILE | 277 | 15.627 | -4.881  | 32.520 | 1.00 | 15.71 | MTGL |
| ATOM | 2181 | CA  | ILE | 277 | 16.558 | -4.864  | 31.399 | 1.00 | 14.72 | MTGL |
| ATOM | 2182 | CB  | ILE | 277 | 17.364 | -6.181  | 31.330 | 1.00 | 14.70 | MTGL |
| ATOM | 2183 | CG2 | ILE | 277 | 18.227 | -6.209  | 30.063 | 1.00 | 14.44 | MTGL |
| ATOM | 2184 | CG1 | ILE | 277 | 18.238 | -6.305  | 32.587 | 1.00 | 14.86 | MTGL |
| ATOM | 2185 | CD1 | ILE | 277 | 18.945 | -7.635  | 32.727 | 1.00 | 14.36 | MTGL |
| ATOM | 2186 | C   | ILE | 277 | 15.832 | -4.643  | 30.081 | 1.00 | 14.58 | MTGL |
| ATOM | 2187 | O   | ILE | 277 | 16.286 | -3.868  | 29.250 | 1.00 | 14.01 | MTGL |
| ATOM | 2188 | N   | THR | 278 | 14.708 | -5.330  | 29.890 | 1.00 | 14.56 | MTGL |
| ATOM | 2189 | CA  | THR | 278 | 13.930 | -5.182  | 28.663 | 1.00 | 15.56 | MTGL |
| ATOM | 2190 | CB  | THR | 278 | 12.724 | -6.159  | 28.635 | 1.00 | 15.82 | MTGL |
| ATOM | 2191 | OG1 | THR | 278 | 13.203 | -7.505  | 28.742 | 1.00 | 16.63 | MTGL |
| ATOM | 2192 | CG2 | THR | 278 | 11.942 | -6.017  | 27.329 | 1.00 | 15.47 | MTGL |
| ATOM | 2193 | C   | THR | 278 | 13.411 | -3.747  | 28.530 | 1.00 | 15.31 | MTGL |
| ATOM | 2194 | O   | THR | 278 | 13.435 | -3.168  | 27.446 | 1.00 | 16.65 | MTGL |
| ATOM | 2195 | N   | ASN | 279 | 12.946 | -3.174  | 29.634 | 1.00 | 15.85 | MTGL |
| ATOM | 2196 | CA  | ASN | 279 | 12.430 | -1.808  | 29.609 | 1.00 | 16.36 | MTGL |
| ATOM | 2197 | CB  | ASN | 279 | 11.743 | -1.475  | 30.939 | 1.00 | 15.56 | MTGL |
| ATOM | 2198 | CG  | ASN | 279 | 10.388 | -2.159  | 31.077 | 1.00 | 17.29 | MTGL |
| ATOM | 2199 | OD1 | ASN | 279 | 9.939  | -2.848  | 30.167 | 1.00 | 15.98 | MTGL |
| ATOM | 2200 | ND2 | ASN | 279 | 9.736  | -1.966  | 32.215 | 1.00 | 17.61 | MTGL |
| ATOM | 2201 | C   | ASN | 279 | 13.520 | -0.783  | 29.304 | 1.00 | 16.68 | MTGL |
| ATOM | 2202 | O   | ASN | 279 | 13.300 | 0.155   | 28.533 | 1.00 | 16.98 | MTGL |
| ATOM | 2203 | N   | VAL | 280 | 14.695 | -0.950  | 29.904 | 1.00 | 16.27 | MTGL |

Fig. 1 cont.

| ATOM | 2204 | CA | VAL | 280 | 15.782 | -0.013 | 29.641 | 1.00 | 15.63 | MTGL |
|------|------|-----|-----|-----|--------|--------|--------|------|-------|------|
| ATOM | 2205 | CB | VAL | 280 | 17.005 | -0.283 | 30.545 | 1.00 | 15.75 | MTGL |
| ATOM | 2206 | CG1 | VAL | 280 | 18.171 | 0.623 | 30.126 | 1.00 | 14.59 | MTGL |
| ATOM | 2207 | CG2 | VAL | 280 | 16.634 | -0.023 | 32.007 | 1.00 | 14.29 | MTGL |
| ATOM | 2208 | C | VAL | 280 | 16.203 | -0.144 | 28.183 | 1.00 | 15.42 | MTGL |
| ATOM | 2209 | O | VAL | 280 | 16.483 | 0.852 | 27.512 | 1.00 | 14.80 | MTGL |
| ATOM | 2210 | N | ALA | 281 | 16.236 | -1.381 | 27.697 | 1.00 | 14.47 | MTGL |
| ATOM | 2211 | CA | ALA | 281 | 16.614 | -1.645 | 26.315 | 1.00 | 15.95 | MTGL |
| ATOM | 2212 | CB | ALA | 281 | 16.573 | -3.147 | 26.035 | 1.00 | 15.85 | MTGL |
| ATOM | 2213 | C | ALA | 281 | 15.662 | -0.922 | 25.369 | 1.00 | 16.21 | MTGL |
| ATOM | 2214 | O | ALA | 281 | 16.087 | -0.290 | 24.403 | 1.00 | 15.33 | MTGL |
| ATOM | 2215 | N | ASN | 282 | 14.369 | -1.018 | 25.653 | 1.00 | 16.95 | MTGL |
| ATOM | 2216 | CA | ASN | 282 | 13.383 | -0.386 | 24.792 | 1.00 | 17.84 | MTGL |
| ATOM | 2217 | CB | ASN | 282 | 12.015 | -1.013 | 25.021 | 1.00 | 19.13 | MTGL |
| ATOM | 2218 | CG | ASN | 282 | 11.924 | -2.398 | 24.400 | 1.00 | 20.19 | MTGL |
| ATOM | 2219 | OD1 | ASN | 282 | 12.393 | -2.605 | 23.289 | 1.00 | 23.04 | MTGL |
| ATOM | 2220 | ND2 | ASN | 282 | 11.328 | -3.341 | 25.108 | 1.00 | 19.74 | MTGL |
| ATOM | 2221 | C | ASN | 282 | 13.337 | 1.124 | 24.910 | 1.00 | 18.52 | MTGL |
| ATOM | 2222 | O | ASN | 282 | 12.841 | 1.806 | 24.011 | 1.00 | 17.57 | MTGL |
| ATOM | 2223 | N | ILE | 283 | 13.851 | 1.651 | 26.015 | 1.00 | 18.29 | MTGL |
| ATOM | 2224 | CA | ILE | 283 | 13.902 | 3.095 | 26.168 | 1.00 | 18.86 | MTGL |
| ATOM | 2225 | CB | ILE | 283 | 14.254 | 3.496 | 27.603 | 1.00 | 19.57 | MTGL |
| ATOM | 2226 | CG2 | ILE | 283 | 14.818 | 4.917 | 27.636 | 1.00 | 20.74 | MTGL |
| ATOM | 2227 | CG1 | ILE | 283 | 13.003 | 3.365 | 28.471 | 1.00 | 21.83 | MTGL |
| ATOM | 2228 | CD1 | ILE | 283 | 13.214 | 3.728 | 29.909 | 1.00 | 25.75 | MTGL |
| ATOM | 2229 | C | ILE | 283 | 14.994 | 3.566 | 25.209 | 1.00 | 17.96 | MTGL |
| ATOM | 2230 | O | ILE | 283 | 14.816 | 4.543 | 24.483 | 1.00 | 17.19 | MTGL |
| ATOM | 2231 | N | VAL | 284 | 16.114 | 2.844 | 25.200 | 1.00 | 17.16 | MTGL |
| ATOM | 2232 | CA | VAL | 284 | 17.236 | 3.164 | 24.321 | 1.00 | 15.86 | MTGL |
| ATOM | 2233 | CB | VAL | 284 | 18.420 | 2.194 | 24.554 | 1.00 | 16.05 | MTGL |
| ATOM | 2234 | CG1 | VAL | 284 | 19.491 | 2.409 | 23.491 | 1.00 | 14.09 | MTGL |
| ATOM | 2235 | CG2 | VAL | 284 | 19.006 | 2.416 | 25.956 | 1.00 | 14.93 | MTGL |
| ATOM | 2236 | C | VAL | 284 | 16.797 | 3.075 | 22.861 | 1.00 | 16.21 | MTGL |
| ATOM | 2237 | O | VAL | 284 | 17.089 | 3.963 | 22.059 | 1.00 | 15.26 | MTGL |
| ATOM | 2238 | N | SER | 285 | 16.086 | 2.004 | 22.519 | 1.00 | 16.71 | MTGL |
| ATOM | 2239 | CA | SER | 285 | 15.618 | 1.813 | 21.145 | 1.00 | 18.87 | MTGL |
| ATOM | 2240 | CB | SER | 285 | 14.977 | 0.429 | 20.979 | 1.00 | 18.71 | MTGL |
| ATOM | 2241 | OG | SER | 285 | 15.954 | -0.595 | 21.082 | 1.00 | 25.57 | MTGL |
| ATOM | 2242 | C | SER | 285 | 14.622 | 2.882 | 20.697 | 1.00 | 18.52 | MTGL |
| ATOM | 2243 | O | SER | 285 | 14.453 | 3.101 | 19.507 | 1.00 | 19.96 | MTGL |
| ATOM | 2244 | N | SER | 286 | 13.964 | 3.544 | 21.644 | 1.00 | 17.61 | MTGL |
| ATOM | 2245 | CA | SER | 286 | 12.993 | 4.574 | 21.295 | 1.00 | 18.49 | MTGL |
| ATOM | 2246 | CB | SER | 286 | 11.970 | 4.754 | 22.421 | 1.00 | 18.70 | MTGL |
| ATOM | 2247 | OG | SER | 286 | 12.505 | 5.533 | 23.483 | 1.00 | 18.21 | MTGL |
| ATOM | 2248 | C | SER | 286 | 13.686 | 5.909 | 21.040 | 1.00 | 18.76 | MTGL |
| ATOM | 2249 | O | SER | 286 | 13.043 | 6.892 | 20.676 | 1.00 | 17.84 | MTGL |
| ATOM | 2250 | N | VAL | 287 | 15.000 | 5.931 | 21.235 | 1.00 | 18.85 | MTGL |
| ATOM | 2251 | CA | VAL | 287 | 15.793 | 7.138 | 21.048 | 1.00 | 17.18 | MTGL |
| ATOM | 2252 | CB | VAL | 287 | 16.866 | 7.267 | 22.158 | 1.00 | 17.69 | MTGL |
| ATOM | 2253 | CG1 | VAL | 287 | 17.764 | 8.477 | 21.890 | 1.00 | 17.29 | MTGL |
| ATOM | 2254 | CG2 | VAL | 287 | 16.189 | 7.399 | 23.512 | 1.00 | 17.29 | MTGL |
| ATOM | 2255 | C | VAL | 287 | 16.493 | 7.144 | 19.702 | 1.00 | 17.44 | MTGL |
| ATOM | 2256 | O | VAL | 287 | 16.979 | 6.112 | 19.241 | 1.00 | 16.36 | MTGL |
| ATOM | 2257 | N | SER | 288 | 16.546 | 8.313 | 19.073 | 1.00 | 18.07 | MTGL |
| ATOM | 2258 | CA | SER | 288 | 17.215 | 8.442 | 17.787 | 1.00 | 18.93 | MTGL |
| ATOM | 2259 | CB | SER | 288 | 17.202 | 9.900 | 17.329 | 1.00 | 19.03 | MTGL |
| ATOM | 2260 | OG | SER | 288 | 17.858 | 10.045 | 16.082 | 1.00 | 21.05 | MTGL |
| ATOM | 2261 | C | SER | 288 | 18.657 | 7.950 | 17.911 | 1.00 | 18.73 | MTGL |

Fig. 1 cont.

| | | | | | | | | | | |
|------|------|-----|-----|-----|--------|--------|--------|------|-------|------|
| ATOM | 2262 | O   | SER | 288 | 19.444 | 8.498  | 18.682 | 1.00 | 18.95 | MTGL |
| ATOM | 2263 | N   | ARG | 289 | 18.984 | 6.915  | 17.145 | 1.00 | 17.81 | MTGL |
| ATOM | 2264 | CA  | ARG | 289 | 20.313 | 6.311  | 17.137 | 1.00 | 18.49 | MTGL |
| ATOM | 2265 | CB  | ARG | 289 | 21.387 | 7.347  | 16.760 | 1.00 | 20.78 | MTGL |
| ATOM | 2266 | CG  | ARG | 289 | 21.128 | 8.067  | 15.429 | 1.00 | 24.72 | MTGL |
| ATOM | 2267 | CD  | ARG | 289 | 22.378 | 8.761  | 14.890 | 1.00 | 26.86 | MTGL |
| ATOM | 2268 | NE  | ARG | 289 | 23.269 | 7.812  | 14.225 | 1.00 | 31.29 | MTGL |
| ATOM | 2269 | CZ  | ARG | 289 | 24.483 | 8.101  | 13.758 | 1.00 | 32.57 | MTGL |
| ATOM | 2270 | NH1 | ARG | 289 | 24.981 | 9.327  | 13.880 | 1.00 | 33.06 | MTGL |
| ATOM | 2271 | NH2 | ARG | 289 | 25.200 | 7.159  | 13.159 | 1.00 | 32.56 | MTGL |
| ATOM | 2272 | C   | ARG | 289 | 20.687 | 5.616  | 18.456 | 1.00 | 17.41 | MTGL |
| ATOM | 2273 | O   | ARG | 289 | 21.865 | 5.493  | 18.785 | 1.00 | 16.35 | MTGL |
| ATOM | 2274 | N   | GLY | 290 | 19.681 | 5.173  | 19.207 | 1.00 | 16.31 | MTGL |
| ATOM | 2275 | CA  | GLY | 290 | 19.944 | 4.449  | 20.442 | 1.00 | 16.82 | MTGL |
| ATOM | 2276 | C   | GLY | 290 | 20.267 | 3.042  | 19.970 | 1.00 | 17.04 | MTGL |
| ATOM | 2277 | O   | GLY | 290 | 19.393 | 2.353  | 19.450 | 1.00 | 16.17 | MTGL |
| ATOM | 2278 | N   | VAL | 291 | 21.502 | 2.595  | 20.159 | 1.00 | 17.31 | MTGL |
| ATOM | 2279 | CA  | VAL | 291 | 21.893 | 1.290  | 19.644 | 1.00 | 17.47 | MTGL |
| ATOM | 2280 | CB  | VAL | 291 | 22.951 | 1.475  | 18.534 | 1.00 | 17.89 | MTGL |
| ATOM | 2281 | CG1 | VAL | 291 | 22.387 | 2.347  | 17.419 | 1.00 | 18.32 | MTGL |
| ATOM | 2282 | CG2 | VAL | 291 | 24.204 | 2.125  | 19.112 | 1.00 | 16.95 | MTGL |
| ATOM | 2283 | C   | VAL | 291 | 22.403 | 0.194  | 20.581 | 1.00 | 18.18 | MTGL |
| ATOM | 2284 | O   | VAL | 291 | 22.610 | -0.933 | 20.133 | 1.00 | 17.39 | MTGL |
| ATOM | 2285 | N   | GLY | 292 | 22.608 | 0.489  | 21.861 | 1.00 | 18.56 | MTGL |
| ATOM | 2286 | CA  | GLY | 292 | 23.117 | -0.559 | 22.730 | 1.00 | 17.86 | MTGL |
| ATOM | 2287 | C   | GLY | 292 | 22.774 | -0.538 | 24.205 | 1.00 | 18.08 | MTGL |
| ATOM | 2288 | O   | GLY | 292 | 22.404 | 0.493  | 24.766 | 1.00 | 17.12 | MTGL |
| ATOM | 2289 | N   | LEU | 293 | 22.913 | -1.708 | 24.824 | 1.00 | 18.07 | MTGL |
| ATOM | 2290 | CA  | LEU | 293 | 22.653 | -1.902 | 26.246 | 1.00 | 18.28 | MTGL |
| ATOM | 2291 | CB  | LEU | 293 | 21.223 | -2.404 | 26.474 | 1.00 | 19.14 | MTGL |
| ATOM | 2292 | CG  | LEU | 293 | 20.858 | -2.808 | 27.910 | 1.00 | 22.33 | MTGL |
| ATOM | 2293 | CD1 | LEU | 293 | 21.047 | -1.625 | 28.842 | 1.00 | 23.17 | MTGL |
| ATOM | 2294 | CD2 | LEU | 293 | 19.410 | -3.278 | 27.965 | 1.00 | 23.54 | MTGL |
| ATOM | 2295 | C   | LEU | 293 | 23.634 | -2.952 | 26.744 | 1.00 | 17.77 | MTGL |
| ATOM | 2296 | O   | LEU | 293 | 23.763 | -4.009 | 26.130 | 1.00 | 17.95 | MTGL |
| ATOM | 2297 | N   | PHE | 294 | 24.322 | -2.658 | 27.847 | 1.00 | 16.70 | MTGL |
| ATOM | 2298 | CA  | PHE | 294 | 25.288 | -3.586 | 28.431 | 1.00 | 16.53 | MTGL |
| ATOM | 2299 | CB  | PHE | 294 | 26.726 | -3.097 | 28.229 | 1.00 | 16.07 | MTGL |
| ATOM | 2300 | CG  | PHE | 294 | 27.199 | -3.136 | 26.800 | 1.00 | 16.47 | MTGL |
| ATOM | 2301 | CD1 | PHE | 294 | 26.792 | -2.164 | 25.890 | 1.00 | 16.58 | MTGL |
| ATOM | 2302 | CD2 | PHE | 294 | 28.069 | -4.137 | 26.368 | 1.00 | 15.29 | MTGL |
| ATOM | 2303 | CE1 | PHE | 294 | 27.241 | -2.188 | 24.571 | 1.00 | 16.35 | MTGL |
| ATOM | 2304 | CE2 | PHE | 294 | 28.523 | -4.170 | 25.050 | 1.00 | 15.62 | MTGL |
| ATOM | 2305 | CZ  | PHE | 294 | 28.110 | -3.192 | 24.150 | 1.00 | 15.75 | MTGL |
| ATOM | 2306 | C   | PHE | 294 | 25.046 | -3.739 | 29.930 | 1.00 | 16.96 | MTGL |
| ATOM | 2307 | O   | PHE | 294 | 25.032 | -2.752 | 30.667 | 1.00 | 17.04 | MTGL |
| ATOM | 2308 | N   | TYR | 295 | 24.855 | -4.977 | 30.374 | 1.00 | 16.03 | MTGL |
| ATOM | 2309 | CA  | TYR | 295 | 24.639 | -5.253 | 31.789 | 1.00 | 15.26 | MTGL |
| ATOM | 2310 | CB  | TYR | 295 | 23.905 | -6.582 | 31.963 | 1.00 | 14.47 | MTGL |
| ATOM | 2311 | CG  | TYR | 295 | 23.323 | -6.755 | 33.344 | 1.00 | 14.21 | MTGL |
| ATOM | 2312 | CD1 | TYR | 295 | 22.033 | -6.312 | 33.637 | 1.00 | 12.09 | MTGL |
| ATOM | 2313 | CE1 | TYR | 295 | 21.512 | -6.421 | 34.918 | 1.00 | 13.83 | MTGL |
| ATOM | 2314 | CD2 | TYR | 295 | 24.080 | -7.316 | 34.372 | 1.00 | 13.69 | MTGL |
| ATOM | 2315 | CE2 | TYR | 295 | 23.566 | -7.431 | 35.662 | 1.00 | 13.74 | MTGL |
| ATOM | 2316 | CZ  | TYR | 295 | 22.284 | -6.979 | 35.930 | 1.00 | 14.39 | MTGL |
| ATOM | 2317 | OH  | TYR | 295 | 21.784 | -7.058 | 37.211 | 1.00 | 15.39 | MTGL |
| ATOM | 2318 | C   | TYR | 295 | 26.033 | -5.346 | 32.410 | 1.00 | 15.23 | MTGL |
| ATOM | 2319 | O   | TYR | 295 | 26.932 | -5.933 | 31.814 | 1.00 | 15.00 | MTGL |

## Fig. 1 cont.

| ATOM | 2320 | N   | TRP | 296 | 26.228 | -4.778  | 33.594 | 1.00 | 14.56 | MTGL |
|------|------|-----|-----|-----|--------|---------|--------|------|-------|------|
| ATOM | 2321 | CA  | TRP | 296 | 27.559 | -4.829  | 34.195 | 1.00 | 15.23 | MTGL |
| ATOM | 2322 | CB  | TRP | 296 | 27.847 | -3.541  | 34.984 | 1.00 | 14.28 | MTGL |
| ATOM | 2323 | CG  | TRP | 296 | 29.306 | -3.370  | 35.309 | 1.00 | 15.53 | MTGL |
| ATOM | 2324 | CD2 | TRP | 296 | 29.918 | -3.408  | 36.611 | 1.00 | 16.19 | MTGL |
| ATOM | 2325 | CE2 | TRP | 296 | 31.309 | -3.221  | 36.424 | 1.00 | 15.45 | MTGL |
| ATOM | 2326 | CE3 | TRP | 296 | 29.428 | -3.583  | 37.916 | 1.00 | 16.72 | MTGL |
| ATOM | 2327 | CD1 | TRP | 296 | 30.321 | -3.168  | 34.418 | 1.00 | 15.37 | MTGL |
| ATOM | 2328 | NE1 | TRP | 296 | 31.526 | -3.077  | 35.079 | 1.00 | 15.66 | MTGL |
| ATOM | 2329 | CZ2 | TRP | 296 | 32.219 | -3.201  | 37.495 | 1.00 | 15.21 | MTGL |
| ATOM | 2330 | CZ3 | TRP | 296 | 30.334 | -3.564  | 38.985 | 1.00 | 16.55 | MTGL |
| ATOM | 2331 | CH2 | TRP | 296 | 31.715 | -3.375  | 38.763 | 1.00 | 16.36 | MTGL |
| ATOM | 2332 | C   | TRP | 296 | 27.842 | -6.029  | 35.097 | 1.00 | 14.61 | MTGL |
| ATOM | 2333 | O   | TRP | 296 | 27.174 | -6.224  | 36.114 | 1.00 | 15.45 | MTGL |
| ATOM | 2334 | N   | GLU | 297 | 28.835 | -6.826  | 34.702 | 1.00 | 14.69 | MTGL |
| ATOM | 2335 | CA  | GLU | 297 | 29.298 | -7.977  | 35.479 | 1.00 | 14.59 | MTGL |
| ATOM | 2336 | CB  | GLU | 297 | 30.125 | -7.465  | 36.661 | 1.00 | 13.64 | MTGL |
| ATOM | 2337 | CG  | GLU | 297 | 31.453 | -6.849  | 36.261 | 1.00 | 14.27 | MTGL |
| ATOM | 2338 | CD  | GLU | 297 | 32.506 | -7.896  | 35.947 | 1.00 | 13.45 | MTGL |
| ATOM | 2339 | OE1 | GLU | 297 | 32.176 | -9.102  | 35.991 | 1.00 | 12.29 | MTGL |
| ATOM | 2340 | OE2 | GLU | 297 | 33.661 | -7.510  | 35.660 | 1.00 | 14.90 | MTGL |
| ATOM | 2341 | C   | GLU | 297 | 28.245 | -8.952  | 36.000 | 1.00 | 15.16 | MTGL |
| ATOM | 2342 | O   | GLU | 297 | 28.177 | -9.219  | 37.205 | 1.00 | 15.61 | MTGL |
| ATOM | 2343 | N   | PRO | 298 | 27.436 | -9.529  | 35.100 | 1.00 | 14.59 | MTGL |
| ATOM | 2344 | CD  | PRO | 298 | 27.545 | -9.487  | 33.631 | 1.00 | 12.84 | MTGL |
| ATOM | 2345 | CA  | PRO | 298 | 26.395 | -10.474 | 35.517 | 1.00 | 14.70 | MTGL |
| ATOM | 2346 | CB  | PRO | 298 | 25.651 | -10.750 | 34.217 | 1.00 | 13.52 | MTGL |
| ATOM | 2347 | CG  | PRO | 298 | 26.765 | -10.716 | 33.213 | 1.00 | 12.86 | MTGL |
| ATOM | 2348 | C   | PRO | 298 | 26.897 | -11.774 | 36.158 | 1.00 | 14.86 | MTGL |
| ATOM | 2349 | O   | PRO | 298 | 26.159 | -12.424 | 36.901 | 1.00 | 14.01 | MTGL |
| ATOM | 2350 | N   | ALA | 299 | 28.143 | -12.147 | 35.875 | 1.00 | 15.30 | MTGL |
| ATOM | 2351 | CA  | ALA | 299 | 28.689 | -13.397 | 36.396 | 1.00 | 16.12 | MTGL |
| ATOM | 2352 | CB  | ALA | 299 | 29.321 | -14.184 | 35.245 | 1.00 | 16.45 | MTGL |
| ATOM | 2353 | C   | ALA | 299 | 29.684 | -13.297 | 37.551 | 1.00 | 16.40 | MTGL |
| ATOM | 2354 | O   | ALA | 299 | 30.281 | -14.303 | 37.934 | 1.00 | 16.31 | MTGL |
| ATOM | 2355 | N   | TRP | 300 | 29.861 | -12.104 | 38.111 | 1.00 | 16.53 | MTGL |
| ATOM | 2356 | CA  | TRP | 300 | 30.804 | -11.911 | 39.218 | 1.00 | 16.99 | MTGL |
| ATOM | 2357 | CB  | TRP | 300 | 31.205 | -10.438 | 39.300 | 1.00 | 15.26 | MTGL |
| ATOM | 2358 | CG  | TRP | 300 | 32.518 | -10.195 | 39.960 | 1.00 | 16.30 | MTGL |
| ATOM | 2359 | CD2 | TRP | 300 | 33.248 | -8.960  | 39.982 | 1.00 | 14.96 | MTGL |
| ATOM | 2360 | CE2 | TRP | 300 | 34.440 | -9.195  | 40.697 | 1.00 | 14.93 | MTGL |
| ATOM | 2361 | CE3 | TRP | 300 | 33.007 | -7.679  | 39.463 | 1.00 | 15.40 | MTGL |
| ATOM | 2362 | CD1 | TRP | 300 | 33.274 | -11.099 | 40.648 | 1.00 | 14.90 | MTGL |
| ATOM | 2363 | NE1 | TRP | 300 | 34.429 | -10.508 | 41.092 | 1.00 | 16.48 | MTGL |
| ATOM | 2364 | CZ2 | TRP | 300 | 35.398 | -8.195  | 40.912 | 1.00 | 13.85 | MTGL |
| ATOM | 2365 | CZ3 | TRP | 300 | 33.960 | -6.678  | 39.678 | 1.00 | 13.88 | MTGL |
| ATOM | 2366 | CH2 | TRP | 300 | 35.143 | -6.949  | 40.398 | 1.00 | 15.26 | MTGL |
| ATOM | 2367 | C   | TRP | 300 | 30.159 | -12.347 | 40.536 | 1.00 | 17.14 | MTGL |
| ATOM | 2368 | O   | TRP | 300 | 29.909 | -11.522 | 41.423 | 1.00 | 16.66 | MTGL |
| ATOM | 2369 | N   | ILE | 301 | 29.907 | -13.645 | 40.670 | 1.00 | 17.69 | MTGL |
| ATOM | 2370 | CA  | ILE | 301 | 29.255 | -14.168 | 41.866 | 1.00 | 19.29 | MTGL |
| ATOM | 2371 | CB  | ILE | 301 | 28.893 | -15.655 | 41.695 | 1.00 | 20.95 | MTGL |
| ATOM | 2372 | CG2 | ILE | 301 | 27.937 | -15.812 | 40.517 | 1.00 | 19.88 | MTGL |
| ATOM | 2373 | CG1 | ILE | 301 | 30.153 | -16.496 | 41.479 | 1.00 | 22.04 | MTGL |
| ATOM | 2374 | CD1 | ILE | 301 | 29.858 | -17.985 | 41.366 | 1.00 | 23.83 | MTGL |
| ATOM | 2375 | C   | ILE | 301 | 29.973 | -13.980 | 43.205 | 1.00 | 19.82 | MTGL |
| ATOM | 2376 | O   | ILE | 301 | 29.325 | -14.022 | 44.249 | 1.00 | 19.53 | MTGL |
| ATOM | 2377 | N   | HIS | 302 | 31.287 | -13.768 | 43.189 | 1.00 | 19.79 | MTGL |

Fig. 1 cont.

| ATOM | 2378 | CA | HIS | 302 | 32.016 | -13.555 | 44.441 | 1.00 | 21.73 | MTGL |
|------|------|-----|-----|-----|--------|---------|--------|------|-------|------|
| ATOM | 2379 | CB | HIS | 302 | 33.464 | -14.042 | 44.317 | 1.00 | 22.38 | MTGL |
| ATOM | 2380 | CG | HIS | 302 | 33.603 | -15.529 | 44.396 | 1.00 | 24.09 | MTGL |
| ATOM | 2381 | CD2 | HIS | 302 | 33.254 | -16.405 | 45.368 | 1.00 | 25.41 | MTGL |
| ATOM | 2382 | ND1 | HIS | 302 | 34.154 | -16.282 | 43.382 | 1.00 | 25.82 | MTGL |
| ATOM | 2383 | CE1 | HIS | 302 | 34.137 | -17.558 | 43.724 | 1.00 | 26.05 | MTGL |
| ATOM | 2384 | NE2 | HIS | 302 | 33.596 | -17.659 | 44.924 | 1.00 | 26.28 | MTGL |
| ATOM | 2385 | C | HIS | 302 | 32.002 | -12.085 | 44.857 | 1.00 | 21.31 | MTGL |
| ATOM | 2386 | O | HIS | 302 | 32.609 | -11.707 | 45.854 | 1.00 | 22.67 | MTGL |
| ATOM | 2387 | N | ASN | 303 | 31.303 | -11.265 | 44.079 | 1.00 | 20.90 | MTGL |
| ATOM | 2388 | CA | ASN | 303 | 31.183 | -9.831 | 44.337 | 1.00 | 20.21 | MTGL |
| ATOM | 2389 | CB | ASN | 303 | 32.200 | -9.074 | 43.473 | 1.00 | 20.27 | MTGL |
| ATOM | 2390 | CG | ASN | 303 | 32.170 | -7.573 | 43.706 | 1.00 | 21.40 | MTGL |
| ATOM | 2391 | OD1 | ASN | 303 | 31.977 | -7.118 | 44.828 | 1.00 | 22.04 | MTGL |
| ATOM | 2392 | ND2 | ASN | 303 | 32.380 | -6.799 | 42.643 | 1.00 | 19.16 | MTGL |
| ATOM | 2393 | C | ASN | 303 | 29.752 | -9.467 | 43.946 | 1.00 | 20.34 | MTGL |
| ATOM | 2394 | O | ASN | 303 | 29.508 | -8.488 | 43.233 | 1.00 | 18.25 | MTGL |
| ATOM | 2395 | N | ALA | 304 | 28.820 | -10.284 | 44.432 | 1.00 | 19.57 | MTGL |
| ATOM | 2396 | CA | ALA | 304 | 27.395 | -10.180 | 44.134 | 1.00 | 19.48 | MTGL |
| ATOM | 2397 | CB | ALA | 304 | 26.612 | -11.157 | 45.017 | 1.00 | 18.17 | MTGL |
| ATOM | 2398 | C | ALA | 304 | 26.731 | -8.813 | 44.182 | 1.00 | 19.61 | MTGL |
| ATOM | 2399 | O | ALA | 304 | 25.909 | -8.505 | 43.323 | 1.00 | 20.70 | MTGL |
| ATOM | 2400 | N | ASN | 305 | 27.050 | -7.999 | 45.181 | 1.00 | 18.88 | MTGL |
| ATOM | 2401 | CA | ASN | 305 | 26.424 | -6.685 | 45.271 | 1.00 | 19.31 | MTGL |
| ATOM | 2402 | CB | ASN | 305 | 26.580 | -6.114 | 46.683 | 1.00 | 19.61 | MTGL |
| ATOM | 2403 | CG | ASN | 305 | 28.024 | -5.847 | 47.048 | 1.00 | 20.60 | MTGL |
| ATOM | 2404 | OD1 | ASN | 305 | 28.868 | -6.747 | 47.014 | 1.00 | 21.53 | MTGL |
| ATOM | 2405 | ND2 | ASN | 305 | 28.318 | -4.606 | 47.403 | 1.00 | 21.29 | MTGL |
| ATOM | 2406 | C | ASN | 305 | 27.018 | -5.723 | 44.240 | 1.00 | 19.61 | MTGL |
| ATOM | 2407 | O | ASN | 305 | 26.522 | -4.611 | 44.041 | 1.00 | 19.33 | MTGL |
| ATOM | 2408 | N | LEU | 306 | 28.088 | -6.160 | 43.587 | 1.00 | 18.26 | MTGL |
| ATOM | 2409 | CA | LEU | 306 | 28.747 | -5.359 | 42.563 | 1.00 | 18.47 | MTGL |
| ATOM | 2410 | CB | LEU | 306 | 27.919 | -5.384 | 41.270 | 1.00 | 17.67 | MTGL |
| ATOM | 2411 | CG | LEU | 306 | 27.771 | -6.764 | 40.612 | 1.00 | 18.35 | MTGL |
| ATOM | 2412 | CD1 | LEU | 306 | 26.888 | -6.670 | 39.372 | 1.00 | 16.49 | MTGL |
| ATOM | 2413 | CD2 | LEU | 306 | 29.144 | -7.300 | 40.238 | 1.00 | 16.40 | MTGL |
| ATOM | 2414 | C | LEU | 306 | 28.994 | -3.915 | 42.990 | 1.00 | 19.28 | MTGL |
| ATOM | 2415 | O | LEU | 306 | 28.698 | -2.981 | 42.241 | 1.00 | 19.04 | MTGL |
| ATOM | 2416 | N | GLY | 307 | 29.529 | -3.740 | 44.196 | 1.00 | 18.62 | MTGL |
| ATOM | 2417 | CA | GLY | 307 | 29.828 | -2.414 | 44.700 | 1.00 | 18.44 | MTGL |
| ATOM | 2418 | C | GLY | 307 | 28.657 | -1.530 | 45.092 | 1.00 | 18.36 | MTGL |
| ATOM | 2419 | O | GLY | 307 | 28.866 | -0.379 | 45.466 | 1.00 | 18.04 | MTGL |
| ATOM | 2420 | N | SER | 308 | 27.435 | -2.047 | 45.020 | 1.00 | 17.93 | MTGL |
| ATOM | 2421 | CA | SER | 308 | 26.256 | -1.256 | 45.380 | 1.00 | 17.81 | MTGL |
| ATOM | 2422 | CB | SER | 308 | 25.134 | -1.480 | 44.361 | 1.00 | 16.84 | MTGL |
| ATOM | 2423 | OG | SER | 308 | 24.555 | -2.759 | 44.528 | 1.00 | 15.76 | MTGL |
| ATOM | 2424 | C | SER | 308 | 25.756 | -1.651 | 46.762 | 1.00 | 18.10 | MTGL |
| ATOM | 2425 | O | SER | 308 | 26.282 | -2.585 | 47.361 | 1.00 | 18.30 | MTGL |
| ATOM | 2426 | N | SER | 309 | 24.735 | -0.947 | 47.250 | 1.00 | 18.76 | MTGL |
| ATOM | 2427 | CA | SER | 309 | 24.157 | -1.220 | 48.560 | 1.00 | 20.76 | MTGL |
| ATOM | 2428 | CB | SER | 309 | 23.424 | 0.022 | 49.092 | 1.00 | 21.48 | MTGL |
| ATOM | 2429 | OG | SER | 309 | 22.304 | 0.358 | 48.283 | 1.00 | 22.88 | MTGL |
| ATOM | 2430 | C | SER | 309 | 23.193 | -2.404 | 48.517 | 1.00 | 22.16 | MTGL |
| ATOM | 2431 | O | SER | 309 | 22.754 | -2.899 | 49.560 | 1.00 | 23.34 | MTGL |
| ATOM | 2432 | N | CYS | 310 | 22.852 | -2.846 | 47.312 | 1.00 | 22.36 | MTGL |
| ATOM | 2433 | CA | CYS | 310 | 21.954 | -3.987 | 47.159 | 1.00 | 23.23 | MTGL |
| ATOM | 2434 | C | CYS | 310 | 22.784 | -5.265 | 47.300 | 1.00 | 23.23 | MTGL |
| ATOM | 2435 | O | CYS | 310 | 23.935 | -5.300 | 46.877 | 1.00 | 25.45 | MTGL |

# Fig. 1 cont.

| ATOM | 2436 | CB | CYS | 310 | 21.275 | -3.945 | 45.793 | 1.00 | 23.30 | MTGL |
|------|------|-----|-----|-----|--------|--------|--------|------|-------|------|
| ATOM | 2437 | SG | CYS | 310 | 19.871 | -2.792 | 45.648 | 1.00 | 24.32 | MTGL |
| ATOM | 2438 | N | ALA | 311 | 22.197 | -6.309 | 47.877 | 1.00 | 21.14 | MTGL |
| ATOM | 2439 | CA | ALA | 311 | 22.903 | -7.564 | 48.110 | 1.00 | 20.13 | MTGL |
| ATOM | 2440 | CB | ALA | 311 | 22.076 | -8.449 | 49.052 | 1.00 | 20.15 | MTGL |
| ATOM | 2441 | C | ALA | 311 | 23.335 | -8.383 | 46.894 | 1.00 | 19.87 | MTGL |
| ATOM | 2442 | O | ALA | 311 | 24.442 | -8.915 | 46.875 | 1.00 | 18.96 | MTGL |
| ATOM | 2443 | N | ASP | 312 | 22.482 | -8.502 | 45.882 | 1.00 | 18.99 | MTGL |
| ATOM | 2444 | CA | ASP | 312 | 22.849 | -9.313 | 44.723 | 1.00 | 19.21 | MTGL |
| ATOM | 2445 | CB | ASP | 312 | 22.346 | -10.747 | 44.931 | 1.00 | 19.01 | MTGL |
| ATOM | 2446 | CG | ASP | 312 | 22.949 | -11.733 | 43.946 | 1.00 | 19.92 | MTGL |
| ATOM | 2447 | OD1 | ASP | 312 | 23.450 | -11.305 | 42.884 | 1.00 | 19.68 | MTGL |
| ATOM | 2448 | OD2 | ASP | 312 | 22.908 | -12.948 | 44.230 | 1.00 | 20.69 | MTGL |
| ATOM | 2449 | C | ASP | 312 | 22.310 | -8.772 | 43.403 | 1.00 | 18.27 | MTGL |
| ATOM | 2450 | O | ASP | 312 | 21.098 | -8.692 | 43.205 | 1.00 | 18.94 | MTGL |
| ATOM | 2451 | N | ASN | 313 | 23.222 | -8.418 | 42.500 | 1.00 | 17.28 | MTGL |
| ATOM | 2452 | CA | ASN | 313 | 22.855 | -7.892 | 41.187 | 1.00 | 17.18 | MTGL |
| ATOM | 2453 | CB | ASN | 313 | 23.478 | -6.507 | 40.962 | 1.00 | 16.90 | MTGL |
| ATOM | 2454 | CG | ASN | 313 | 22.860 | -5.440 | 41.835 | 1.00 | 17.53 | MTGL |
| ATOM | 2455 | OD1 | ASN | 313 | 21.636 | -5.293 | 41.879 | 1.00 | 20.07 | MTGL |
| ATOM | 2456 | ND2 | ASN | 313 | 23.704 | -4.677 | 42.529 | 1.00 | 16.34 | MTGL |
| ATOM | 2457 | C | ASN | 313 | 23.305 | -8.809 | 40.053 | 1.00 | 17.15 | MTGL |
| ATOM | 2458 | O | ASN | 313 | 23.190 | -8.452 | 38.881 | 1.00 | 17.24 | MTGL |
| ATOM | 2459 | N | THR | 314 | 23.826 | -9.982 | 40.391 | 1.00 | 15.74 | MTGL |
| ATOM | 2460 | CA | THR | 314 | 24.289 | -10.903 | 39.365 | 1.00 | 15.54 | MTGL |
| ATOM | 2461 | CB | THR | 314 | 25.226 | -11.977 | 39.953 | 1.00 | 15.83 | MTGL |
| ATOM | 2462 | OG1 | THR | 314 | 24.502 | -12.779 | 40.894 | 1.00 | 16.12 | MTGL |
| ATOM | 2463 | CG2 | THR | 314 | 26.418 | -11.322 | 40.651 | 1.00 | 14.76 | MTGL |
| ATOM | 2464 | C | THR | 314 | 23.130 | -11.604 | 38.657 | 1.00 | 16.42 | MTGL |
| ATOM | 2465 | O | THR | 314 | 21.972 | -11.525 | 39.087 | 1.00 | 15.23 | MTGL |
| ATOM | 2466 | N | MET | 315 | 23.453 | -12.273 | 37.555 | 1.00 | 16.30 | MTGL |
| ATOM | 2467 | CA | MET | 315 | 22.458 | -13.006 | 36.776 | 1.00 | 17.57 | MTGL |
| ATOM | 2468 | CB | MET | 315 | 22.390 | -12.447 | 35.350 | 1.00 | 16.92 | MTGL |
| ATOM | 2469 | CG | MET | 315 | 21.934 | -10.997 | 35.281 | 1.00 | 16.10 | MTGL |
| ATOM | 2470 | SD | MET | 315 | 21.871 | -10.343 | 33.592 | 1.00 | 18.97 | MTGL |
| ATOM | 2471 | CE | MET | 315 | 20.232 | -10.916 | 33.083 | 1.00 | 14.39 | MTGL |
| ATOM | 2472 | C | MET | 315 | 22.820 | -14.492 | 36.753 | 1.00 | 17.49 | MTGL |
| ATOM | 2473 | O | MET | 315 | 22.404 | -15.234 | 35.871 | 1.00 | 17.40 | MTGL |
| ATOM | 2474 | N | PHE | 316 | 23.614 | -14.905 | 37.736 | 1.00 | 17.70 | MTGL |
| ATOM | 2475 | CA | PHE | 316 | 24.050 | -16.291 | 37.879 | 1.00 | 18.51 | MTGL |
| ATOM | 2476 | CB | PHE | 316 | 25.521 | -16.451 | 37.482 | 1.00 | 16.98 | MTGL |
| ATOM | 2477 | CG | PHE | 316 | 25.760 | -16.485 | 35.995 | 1.00 | 17.56 | MTGL |
| ATOM | 2478 | CD1 | PHE | 316 | 25.616 | -15.337 | 35.220 | 1.00 | 17.13 | MTGL |
| ATOM | 2479 | CD2 | PHE | 316 | 26.124 | -17.671 | 35.370 | 1.00 | 16.95 | MTGL |
| ATOM | 2480 | CE1 | PHE | 316 | 25.845 | -15.370 | 33.845 | 1.00 | 17.76 | MTGL |
| ATOM | 2481 | CE2 | PHE | 316 | 26.355 | -17.717 | 33.993 | 1.00 | 17.39 | MTGL |
| ATOM | 2482 | CZ | PHE | 316 | 26.212 | -16.566 | 33.227 | 1.00 | 16.28 | MTGL |
| ATOM | 2483 | C | PHE | 316 | 23.891 | -16.679 | 39.344 | 1.00 | 19.70 | MTGL |
| ATOM | 2484 | O | PHE | 316 | 23.980 | -15.825 | 40.229 | 1.00 | 19.34 | MTGL |
| ATOM | 2485 | N | SER | 317 | 23.659 | -17.963 | 39.598 | 1.00 | 19.30 | MTGL |
| ATOM | 2486 | CA | SER | 317 | 23.495 | -18.444 | 40.963 | 1.00 | 20.50 | MTGL |
| ATOM | 2487 | CB | SER | 317 | 22.894 | -19.853 | 40.972 | 1.00 | 19.80 | MTGL |
| ATOM | 2488 | OG | SER | 317 | 23.832 | -20.798 | 40.484 | 1.00 | 18.89 | MTGL |
| ATOM | 2489 | C | SER | 317 | 24.860 | -18.479 | 41.633 | 1.00 | 20.89 | MTGL |
| ATOM | 2490 | O | SER | 317 | 25.895 | -18.352 | 40.973 | 1.00 | 19.59 | MTGL |
| ATOM | 2491 | N | GLN | 318 | 24.857 | -18.659 | 42.946 | 1.00 | 21.68 | MTGL |
| ATOM | 2492 | CA | GLN | 318 | 26.104 | -18.711 | 43.685 | 1.00 | 22.69 | MTGL |
| ATOM | 2493 | CB | GLN | 318 | 25.813 | -18.649 | 45.186 | 1.00 | 23.06 | MTGL |

Fig. 1 cont.

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ATOM   2494  CG  GLN  318     25.363 -17.254  45.625  1.00 24.34      MTGL
ATOM   2495  CD  GLN  318     26.459 -16.209  45.445  1.00 25.12      MTGL
ATOM   2496  OE1 GLN  318     27.473 -16.241  46.142  1.00 27.51      MTGL
ATOM   2497  NE2 GLN  318     26.266 -15.287  44.503  1.00 23.16      MTGL
ATOM   2498  C   GLN  318     26.920 -19.947  43.315  1.00 22.71      MTGL
ATOM   2499  O   GLN  318     28.095 -20.052  43.662  1.00 24.10      MTGL
ATOM   2500  N   SER  319     26.307 -20.875  42.588  1.00 22.97      MTGL
ATOM   2501  CA  SER  319     27.022 -22.074  42.160  1.00 23.61      MTGL
ATOM   2502  CB  SER  319     26.112 -23.306  42.235  1.00 24.83      MTGL
ATOM   2503  OG  SER  319     24.914 -23.111  41.500  1.00 28.30      MTGL
ATOM   2504  C   SER  319     27.553 -21.900  40.737  1.00 23.21      MTGL
ATOM   2505  O   SER  319     28.158 -22.814  40.180  1.00 23.75      MTGL
ATOM   2506  N   GLY  320     27.315 -20.726  40.153  1.00 22.56      MTGL
ATOM   2507  CA  GLY  320     27.798 -20.439  38.811  1.00 22.10      MTGL
ATOM   2508  C   GLY  320     26.851 -20.771  37.670  1.00 22.30      MTGL
ATOM   2509  O   GLY  320     27.262 -20.809  36.504  1.00 22.30      MTGL
ATOM   2510  N   GLN  321     25.582 -21.009  37.984  1.00 21.21      MTGL
ATOM   2511  CA  GLN  321     24.618 -21.337  36.941  1.00 21.36      MTGL
ATOM   2512  CB  GLN  321     23.652 -22.415  37.426  1.00 23.27      MTGL
ATOM   2513  CG  GLN  321     22.649 -22.855  36.371  1.00 24.43      MTGL
ATOM   2514  CD  GLN  321     21.803 -24.021  36.833  1.00 26.48      MTGL
ATOM   2515  OE1 GLN  321     22.320 -25.009  37.347  1.00 27.39      MTGL
ATOM   2516  NE2 GLN  321     20.497 -23.920  36.641  1.00 27.02      MTGL
ATOM   2517  C   GLN  321     23.826 -20.121  36.483  1.00 20.04      MTGL
ATOM   2518  O   GLN  321     23.289 -19.371  37.291  1.00 19.56      MTGL
ATOM   2519  N   ALA  322     23.755 -19.939  35.172  1.00 20.60      MTGL
ATOM   2520  CA  ALA  322     23.028 -18.817  34.596  1.00 20.07      MTGL
ATOM   2521  CB  ALA  322     23.129 -18.864  33.079  1.00 18.41      MTGL
ATOM   2522  C   ALA  322     21.565 -18.855  35.017  1.00 20.05      MTGL
ATOM   2523  O   ALA  322     20.921 -19.901  34.945  1.00 19.07      MTGL
ATOM   2524  N   LEU  323     21.052 -17.713  35.464  0.50 19.28      MTGL
ATOM   2525  CA  LEU  323     19.658 -17.611  35.878  0.50 19.33      MTGL
ATOM   2526  CB  LEU  323     19.470 -16.426  36.830  0.50 18.12      MTGL
ATOM   2527  CG  LEU. 323     20.241 -16.493  38.152  0.50 17.16      MTGL
ATOM   2528  CD1 LEU  323     19.944 -15.244  38.979  0.50 16.83      MTGL
ATOM   2529  CD2 LEU  323     19.844 -17.758  38.920  0.50 16.13      MTGL
ATOM   2530  C   LEU  323     18.779 -17.431  34.645  0.50 19.86      MTGL
ATOM   2531  O   LEU  323     19.270 -17.113  33.561  0.50 19.75      MTGL
ATOM   2532  N   SER  324     17.477 -17.630  34.817  1.00 21.01      MTGL
ATOM   2533  CA  SER  324     16.524 -17.511  33.719  1.00 21.34      MTGL
ATOM   2534  CB  SER  324     15.114 -17.827  34.220  1.00 21.65      MTGL
ATOM   2535  OG  SER  324     14.713 -16.887  35.202  1.00 22.41      MTGL
ATOM   2536  C   SER  324     16.529 -16.130  33.075  1.00 21.33      MTGL
ATOM   2537  O   SER  324     16.159 -15.980  31.913  1.00 20.59      MTGL
ATOM   2538  N   SER  325     16.955 -15.123  33.830  1.00 20.04      MTGL
ATOM   2539  CA  SER  325     16.984 -13.759  33.321  1.00 20.07      MTGL
ATOM   2540  CB  SER  325     17.227 -12.780  34.476  1.00 19.69      MTGL
ATOM   2541  OG  SER  325     18.417 -13.106  35.172  1.00 17.73      MTGL
ATOM   2542  C   SER  325     18.012 -13.515  32.213  1.00 20.16      MTGL
ATOM   2543  O   SER  325     17.892 -12.549  31.460  1.00 19.87      MTGL
ATOM   2544  N   LEU  326     19.010 -14.388  32.104  1.00 19.54      MTGL
ATOM   2545  CA  LEU  326     20.048 -14.230  31.085  1.00 19.73      MTGL
ATOM   2546  CB  LEU  326     21.126 -15.314  31.236  1.00 20.49      MTGL
ATOM   2547  CG  LEU  326     22.606 -14.910  31.307  1.00 22.10      MTGL
ATOM   2548  CD1 LEU  326     23.433 -15.966  30.587  1.00 21.95      MTGL
ATOM   2549  CD2 LEU  326     22.848 -13.551  30.678  1.00 22.81      MTGL
ATOM   2550  C   LEU  326     19.519 -14.274  29.646  1.00 19.72      MTGL
ATOM   2551  O   LEU  326     20.094 -13.655  28.754  1.00 19.08      MTGL
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# Fig. 1 cont.

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ATOM   2552  N    SER  327     18.439 -15.015  29.412  1.00 18.98      MTGL
ATOM   2553  CA   SER  327     17.875 -15.133  28.067  1.00 18.71      MTGL
ATOM   2554  CB   SER  327     16.861 -16.271  28.023  1.00 17.52      MTGL
ATOM   2555  OG   SER  327     15.740 -15.947  28.825  1.00 16.77      MTGL
ATOM   2556  C    SER  327     17.191 -13.851  27.585  1.00 18.81      MTGL
ATOM   2557  O    SER  327     16.698 -13.795  26.459  1.00 18.63      MTGL
ATOM   2558  N    VAL  328     17.140 -12.836  28.440  1.00 18.22      MTGL
ATOM   2559  CA   VAL  328     16.517 -11.573  28.066  1.00 18.51      MTGL
ATOM   2560  CB   VAL  328     16.590 -10.545  29.223  1.00 19.11      MTGL
ATOM   2561  CG1  VAL  328     18.046 -10.177  29.509  1.00 17.14      MTGL
ATOM   2562  CG2  VAL  328     15.777  -9.304  28.868  1.00 19.04      MTGL
ATOM   2563  C    VAL  328     17.210 -10.983  26.839  1.00 19.25      MTGL
ATOM   2564  O    VAL  328     16.589 -10.285  26.039  1.00 18.81      MTGL
ATOM   2565  N    PHE  329     18.498 -11.273  26.685  1.00 20.22      MTGL
ATOM   2566  CA   PHE  329     19.258 -10.752  25.550  1.00 22.10      MTGL
ATOM   2567  CB   PHE  329     20.752 -10.989  25.774  1.00 21.20      MTGL
ATOM   2568  CG   PHE  329     21.307 -10.211  26.929  1.00 21.71      MTGL
ATOM   2569  CD1  PHE  329     21.525  -8.842  26.814  1.00 21.66      MTGL
ATOM   2570  CD2  PHE  329     21.551 -10.831  28.151  1.00 20.67      MTGL
ATOM   2571  CE1  PHE  329     21.979  -8.099  27.901  1.00 22.16      MTGL
ATOM   2572  CE2  PHE  329     22.003 -10.098  29.240  1.00 22.03      MTGL
ATOM   2573  CZ   PHE  329     22.215  -8.728  29.114  1.00 22.57      MTGL
ATOM   2574  C    PHE  329     18.815 -11.340  24.212  1.00 23.27      MTGL
ATOM   2575  O    PHE  329     19.267 -10.904  23.152  1.00 23.56      MTGL
ATOM   2576  N    GLN  330     17.927 -12.326  24.267  1.00 23.16      MTGL
ATOM   2577  CA   GLN  330     17.402 -12.950  23.058  1.00 24.83      MTGL
ATOM   2578  CB   GLN  330     16.994 -14.403  23.333  1.00 25.48      MTGL
ATOM   2579  CG   GLN  330     18.138 -15.371  23.573  1.00 25.89      MTGL
ATOM   2580  CD   GLN  330     17.648 -16.773  23.894  1.00 27.09      MTGL
ATOM   2581  OE1  GLN  330     18.390 -17.748  23.750  1.00 29.08      MTGL
ATOM   2582  NE2  GLN  330     16.400 -16.882  24.343  1.00 24.64      MTGL
ATOM   2583  C    GLN  330     16.157 -12.198  22.596  1.00 25.46      MTGL
ATOM   2584  O    GLN  330     15.651 -12.439  21.502  1.00 25.45      MTGL
ATOM   2585  N    ARG  331     15.669 -11.282  23.426  1.00 25.05      MTGL
ATOM   2586  CA   ARG  331     14.443 -10.573  23.094  1.00 25.37      MTGL
ATOM   2587  CB   ARG  331     13.356 -10.991  24.087  1.00 24.60      MTGL
ATOM   2588  CG   ARG  331     13.223 -12.507  24.246  1.00 25.96      MTGL
ATOM   2589  CD   ARG  331     12.110 -12.882  25.220  1.00 26.44      MTGL
ATOM   2590  NE   ARG  331     12.400 -12.493  26.600  1.00 27.25      MTGL
ATOM   2591  CZ   ARG  331     13.123 -13.218  27.451  1.00 27.98      MTGL
ATOM   2592  NH1  ARG  331     13.637 -14.383  27.073  1.00 26.83      MTGL
ATOM   2593  NH2  ARG  331     13.329 -12.777  28.683  1.00 26.92      MTGL
ATOM   2594  C    ARG  331     14.506  -9.049  23.017  1.00 25.38      MTGL
ATOM   2595  O    ARG  331     13.468  -8.391  23.085  1.00 25.25      MTGL
ATOM   2596  N    ILE  332     15.703  -8.487  22.863  1.00 25.52      MTGL
ATOM   2597  CA   ILE  332     15.847  -7.035  22.779  1.00 26.69      MTGL
ATOM   2598  CB   ILE  332     16.510  -6.459  24.049  1.00 26.08      MTGL
ATOM   2599  CG2  ILE  332     15.646  -6.765  25.269  1.00 25.81      MTGL
ATOM   2600  CG1  ILE  332     17.912  -7.047  24.224  1.00 25.06      MTGL
ATOM   2601  CD1  ILE  332     18.663  -6.506  25.425  1.00 23.51      MTGL
ATOM   2602  C    ILE  332     16.664  -6.599  21.567  1.00 27.88      MTGL
ATOM   2603  O    ILE  332     17.171  -7.485  20.855  1.00 28.65      MTGL
ATOM   2604  OXT  ILE  332     16.787  -5.372  21.344  1.00 30.38      MTGL
END
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# Fig. 1 cont.

| HEADER | | | | | | | | | | HIGL |
|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1 | CB | ALA | 1 | 6.247 | 74.348 | 114.849 | 1.00 | 27.43 | HIGL |
| ATOM | 2 | C | ALA | 1 | 7.283 | 72.458 | 113.617 | 1.00 | 26.21 | HIGL |
| ATOM | 3 | O | ALA | 1 | 6.683 | 72.007 | 112.638 | 1.00 | 26.69 | HIGL |
| ATOM | 4 | N | ALA | 1 | 7.237 | 74.771 | 112.633 | 1.00 | 26.59 | HIGL |
| ATOM | 5 | CA | ALA | 1 | 7.343 | 73.961 | 113.883 | 1.00 | 26.86 | HIGL |
| ATOM | 6 | N | LEU | 2 | 7.883 | 71.693 | 114.524 | 1.00 | 24.15 | HIGL |
| ATOM | 7 | CA | LEU | 2 | 7.971 | 70.244 | 114.405 | 1.00 | 22.16 | HIGL |
| ATOM | 8 | CB | LEU | 2 | 8.883 | 69.700 | 115.498 | 1.00 | 21.06 | HIGL |
| ATOM | 9 | CG | LEU | 2 | 10.274 | 70.334 | 115.565 | 1.00 | 20.32 | HIGL |
| ATOM | 10 | CD1 | LEU | 2 | 10.966 | 69.921 | 116.848 | 1.00 | 19.78 | HIGL |
| ATOM | 11 | CD2 | LEU | 2 | 11.076 | 69.921 | 114.346 | 1.00 | 20.05 | HIGL |
| ATOM | 12 | C | LEU | 2 | 6.663 | 69.471 | 114.429 | 1.00 | 22.53 | HIGL |
| ATOM | 13 | O | LEU | 2 | 5.748 | 69.767 | 115.202 | 1.00 | 23.10 | HIGL |
| ATOM | 14 | N | GLN | 3 | 6.597 | 68.456 | 113.576 | 1.00 | 21.51 | HIGL |
| ATOM | 15 | CA | GLN | 3 | 5.430 | 67.601 | 113.493 | 1.00 | 20.06 | HIGL |
| ATOM | 16 | CB | GLN | 3 | 5.435 | 66.837 | 112.175 | 1.00 | 18.80 | HIGL |
| ATOM | 17 | CG | GLN | 3 | 4.157 | 66.084 | 111.909 | 1.00 | 19.14 | HIGL |
| ATOM | 18 | CD | GLN | 3 | 4.246 | 65.213 | 110.680 | 1.00 | 19.73 | HIGL |
| ATOM | 19 | OE1 | GLN | 3 | 4.884 | 65.577 | 109.689 | 1.00 | 21.27 | HIGL |
| ATOM | 20 | NE2 | GLN | 3 | 3.594 | 64.062 | 110.728 | 1.00 | 18.71 | HIGL |
| ATOM | 21 | C | GLN | 3 | 5.504 | 66.609 | 114.644 | 1.00 | 19.78 | HIGL |
| ATOM | 22 | O | GLN | 3 | 4.513 | 66.342 | 115.324 | 1.00 | 20.14 | HIGL |
| ATOM | 23 | N | TYR | 4 | 6.696 | 66.060 | 114.849 | 1.00 | 19.50 | HIGL |
| ATOM | 24 | CA | TYR | 4 | 6.920 | 65.083 | 115.902 | 1.00 | 19.32 | HIGL |
| ATOM | 25 | CB | TYR | 4 | 7.614 | 63.849 | 115.328 | 1.00 | 18.96 | HIGL |
| ATOM | 26 | CG | TYR | 4 | 6.913 | 63.222 | 114.145 | 1.00 | 19.19 | HIGL |
| ATOM | 27 | CD1 | TYR | 4 | 5.639 | 62.669 | 114.271 | 1.00 | 19.50 | HIGL |
| ATOM | 28 | CE1 | TYR | 4 | 5.019 | 62.033 | 113.199 | 1.00 | 18.39 | HIGL |
| ATOM | 29 | CD2 | TYR | 4 | 7.546 | 63.131 | 112.909 | 1.00 | 19.30 | HIGL |
| ATOM | 30 | CE2 | TYR | 4 | 6.935 | 62.497 | 111.831 | 1.00 | 19.42 | HIGL |
| ATOM | 31 | CZ | TYR | 4 | 5.672 | 61.947 | 111.984 | 1.00 | 19.38 | HIGL |
| ATOM | 32 | OH | TYR | 4 | 5.083 | 61.288 | 110.922 | 1.00 | 18.91 | HIGL |
| ATOM | 33 | C | TYR | 4 | 7.790 | 65.686 | 117.000 | 1.00 | 19.57 | HIGL |
| ATOM | 34 | O | TYR | 4 | 8.954 | 66.022 | 116.776 | 1.00 | 19.37 | HIGL |
| ATOM | 35 | N | LYS | 5 | 7.220 | 65.845 | 118.185 | 1.00 | 19.13 | HIGL |
| ATOM | 36 | CA | LYS | 5 | 7.980 | 66.388 | 119.293 | 1.00 | 19.83 | HIGL |
| ATOM | 37 | CB | LYS | 5 | 7.666 | 67.874 | 119.495 | 1.00 | 21.28 | HIGL |
| ATOM | 38 | CG | LYS | 5 | 6.198 | 68.219 | 119.599 | 1.00 | 23.14 | HIGL |
| ATOM | 39 | CD | LYS | 5 | 6.031 | 69.730 | 119.695 | 1.00 | 25.10 | HIGL |
| ATOM | 40 | CE | LYS | 5 | 4.563 | 70.143 | 119.714 | 1.00 | 25.68 | HIGL |
| ATOM | 41 | NZ | LYS | 5 | 4.438 | 71.621 | 119.884 | 1.00 | 27.35 | HIGL |
| ATOM | 42 | C | LYS | 5 | 7.661 | 65.589 | 120.539 | 1.00 | 19.09 | HIGL |
| ATOM | 43 | O | LYS | 5 | 6.537 | 65.616 | 121.043 | 1.00 | 20.34 | HIGL |
| ATOM | 44 | N | GLY | 6 | 8.653 | 64.858 | 121.027 | 1.00 | 17.54 | HIGL |
| ATOM | 45 | CA | GLY | 6 | 8.428 | 64.050 | 122.203 | 1.00 | 16.41 | HIGL |
| ATOM | 46 | C | GLY | 6 | 9.685 | 63.574 | 122.897 | 1.00 | 15.75 | HIGL |
| ATOM | 47 | O | GLY | 6 | 10.779 | 64.112 | 122.698 | 1.00 | 15.49 | HIGL |
| ATOM | 48 | N | VAL | 7 | 9.518 | 62.548 | 123.721 | 1.00 | 14.73 | HIGL |
| ATOM | 49 | CA | VAL | 7 | 10.623 | 61.996 | 124.470 | 1.00 | 14.42 | HIGL |
| ATOM | 50 | CB | VAL | 7 | 10.518 | 62.373 | 125.963 | 1.00 | 15.12 | HIGL |
| ATOM | 51 | CG1 | VAL | 7 | 10.337 | 63.879 | 126.121 | 1.00 | 15.55 | HIGL |
| ATOM | 52 | CG2 | VAL | 7 | 9.361 | 61.620 | 126.605 | 1.00 | 14.47 | HIGL |
| ATOM | 53 | C | VAL | 7 | 10.629 | 60.481 | 124.392 | 1.00 | 13.95 | HIGL |
| ATOM | 54 | O | VAL | 7 | 9.650 | 59.863 | 123.979 | 1.00 | 13.25 | HIGL |
| ATOM | 55 | N | ASP | 8 | 11.753 | 59.895 | 124.784 | 1.00 | 13.51 | HIGL |
| ATOM | 56 | CA | ASP | 8 | 11.863 | 58.452 | 124.844 | 1.00 | 13.71 | HIGL |
| ATOM | 57 | CB | ASP | 8 | 13.263 | 57.981 | 124.473 | 1.00 | 13.57 | HIGL |
| ATOM | 58 | CG | ASP | 8 | 13.354 | 56.480 | 124.393 | 1.00 | 13.68 | HIGL |
| ATOM | 59 | OD1 | ASP | 8 | 12.912 | 55.814 | 125.353 | 1.00 | 13.24 | HIGL |
| ATOM | 60 | OD2 | ASP | 8 | 13.861 | 55.967 | 123.373 | 1.00 | 14.72 | HIGL |
| ATOM | 61 | C | ASP | 8 | 11.626 | 58.233 | 126.324 | 1.00 | 13.84 | HIGL |
| ATOM | 62 | O | ASP | 8 | 12.391 | 58.735 | 127.156 | 1.00 | 13.94 | HIGL |
| ATOM | 63 | N | TRP | 9 | 10.562 | 57.510 | 126.658 | 1.00 | 13.89 | HIGL |
| ATOM | 64 | CA | TRP | 9 | 10.207 | 57.280 | 128.059 | 1.00 | 13.87 | HIGL |

## Fig. 2

| ATOM | 65 | CB | TRP | 9 | 8.822 | 57.889 | 128.324 | 1.00 | 11.91 | HIGL |
|------|-----|------|-----|----|--------|--------|---------|------|-------|------|
| ATOM | 66 | CG | TRP | 9 | 7.684 | 57.044 | 127.823 | 1.00 | 12.26 | HIGL |
| ATOM | 67 | CD2 | TRP | 9 | 6.406 | 56.867 | 128.448 | 1.00 | 12.11 | HIGL |
| ATOM | 68 | CE2 | TRP | 9 | 5.670 | 55.963 | 127.647 | 1.00 | 12.19 | HIGL |
| ATOM | 69 | CE3 | TRP | 9 | 5.809 | 57.383 | 129.609 | 1.00 | 11.70 | HIGL |
| ATOM | 70 | CD1 | TRP | 9 | 7.668 | 56.268 | 126.696 | 1.00 | 11.92 | HIGL |
| ATOM | 71 | NE1 | TRP | 9 | 6.466 | 55.614 | 126.586 | 1.00 | 11.76 | HIGL |
| ATOM | 72 | CZ2 | TRP | 9 | 4.365 | 55.562 | 127.968 | 1.00 | 11.52 | HIGL |
| ATOM | 73 | CZ3 | TRP | 9 | 4.510 | 56.986 | 129.930 | 1.00 | 11.57 | HIGL |
| ATOM | 74 | CH2 | TRP | 9 | 3.804 | 56.085 | 129.111 | 1.00 | 11.64 | HIGL |
| ATOM | 75 | C | TRP | 9 | 10.212 | 55.798 | 128.440 | 1.00 | 14.10 | HIGL |
| ATOM | 76 | O | TRP | 9 | 9.551 | 55.392 | 129.392 | 1.00 | 15.49 | HIGL |
| ATOM | 77 | N | SER | 10 | 10.984 | 55.002 | 127.713 | 1.00 | 14.17 | HIGL |
| ATOM | 78 | CA | SER | 10 | 11.051 | 53.561 | 127.939 | 1.00 | 14.00 | HIGL |
| ATOM | 79 | CB | SER | 10 | 12.154 | 52.958 | 127.056 | 1.00 | 14.22 | HIGL |
| ATOM | 80 | OG | SER | 10 | 11.946 | 53.282 | 125.685 | 1.00 | 12.67 | HIGL |
| ATOM | 81 | C | SER | 10 | 11.232 | 53.095 | 129.385 | 1.00 | 13.46 | HIGL |
| ATOM | 82 | O | SER | 10 | 10.652 | 52.096 | 129.794 | 1.00 | 13.12 | HIGL |
| ATOM | 83 | N | SER | 11 | 12.021 | 53.821 | 130.162 | 1.00 | 13.49 | HIGL |
| ATOM | 84 | CA | SER | 11 | 12.281 | 53.437 | 131.542 | 1.00 | 13.65 | HIGL |
| ATOM | 85 | CB | SER | 11 | 13.490 | 54.200 | 132.051 | 1.00 | 12.96 | HIGL |
| ATOM | 86 | OG | SER | 11 | 13.175 | 55.576 | 132.142 | 1.00 | 11.73 | HIGL |
| ATOM | 87 | C | SER | 11 | 11.134 | 53.664 | 132.524 | 1.00 | 15.06 | HIGL |
| ATOM | 88 | O | SER | 11 | 11.192 | 53.198 | 133.667 | 1.00 | 15.59 | HIGL |
| ATOM | 89 | N | VAL | 12 | 10.090 | 54.357 | 132.089 | 1.00 | 15.52 | HIGL |
| ATOM | 90 | CA | VAL | 12 | 8.987 | 54.682 | 132.983 | 1.00 | 16.34 | HIGL |
| ATOM | 91 | CB | VAL | 12 | 7.793 | 55.248 | 132.197 | 1.00 | 16.01 | HIGL |
| ATOM | 92 | CG1 | VAL | 12 | 7.264 | 54.205 | 131.248 | 1.00 | 16.29 | HIGL |
| ATOM | 93 | CG2 | VAL | 12 | 6.714 | 55.720 | 133.159 | 1.00 | 15.28 | HIGL |
| ATOM | 94 | C | VAL | 12 | 8.485 | 53.594 | 133.945 | 1.00 | 17.29 | HIGL |
| ATOM | 95 | O | VAL | 12 | 8.361 | 53.855 | 135.143 | 1.00 | 18.04 | HIGL |
| ATOM | 96 | N | MET | 13 | 8.197 | 52.390 | 133.457 | 1.00 | 17.84 | HIGL |
| ATOM | 97 | CA | MET | 13 | 7.695 | 51.346 | 134.355 | 1.00 | 17.96 | HIGL |
| ATOM | 98 | CB | MET | 13 | 7.044 | 50.203 | 133.568 | 1.00 | 17.95 | HIGL |
| ATOM | 99 | CG | MET | 13 | 5.703 | 50.579 | 132.968 | 1.00 | 19.53 | HIGL |
| ATOM | 100 | SD | MET | 13 | 4.678 | 49.147 | 132.593 | 1.00 | 23.13 | HIGL |
| ATOM | 101 | CE | MET | 13 | 5.559 | 48.452 | 131.185 | 1.00 | 23.08 | HIGL |
| ATOM | 102 | C | MET | 13 | 8.756 | 50.788 | 135.290 | 1.00 | 17.76 | HIGL |
| ATOM | 103 | O | MET | 13 | 8.456 | 50.415 | 136.420 | 1.00 | 17.26 | HIGL |
| ATOM | 104 | N | VAL | 14 | 9.994 | 50.723 | 134.817 | 1.00 | 17.91 | HIGL |
| ATOM | 105 | CA | VAL | 14 | 11.082 | 50.225 | 135.640 | 1.00 | 17.21 | HIGL |
| ATOM | 106 | CB | VAL | 14 | 12.413 | 50.169 | 134.845 | 1.00 | 16.85 | HIGL |
| ATOM | 107 | CG1 | VAL | 14 | 13.559 | 49.837 | 135.761 | 1.00 | 13.37 | HIGL |
| ATOM | 108 | CG2 | VAL | 14 | 12.311 | 49.128 | 133.741 | 1.00 | 15.66 | HIGL |
| ATOM | 109 | C | VAL | 14 | 11.212 | 51.187 | 136.809 | 1.00 | 17.76 | HIGL |
| ATOM | 110 | O | VAL | 14 | 11.455 | 50.774 | 137.945 | 1.00 | 18.17 | HIGL |
| ATOM | 111 | N | GLU | 15 | 11.031 | 52.473 | 136.533 | 1.00 | 18.10 | HIGL |
| ATOM | 112 | CA | GLU | 15 | 11.120 | 53.476 | 137.586 | 1.00 | 19.10 | HIGL |
| ATOM | 113 | CB | GLU | 15 | 11.207 | 54.881 | 136.991 | 1.00 | 19.32 | HIGL |
| ATOM | 114 | CG | GLU | 15 | 12.554 | 55.178 | 136.365 | 1.00 | 20.08 | HIGL |
| ATOM | 115 | CD | GLU | 15 | 13.676 | 55.158 | 137.383 | 1.00 | 21.57 | HIGL |
| ATOM | 116 | OE1 | GLU | 15 | 13.838 | 54.131 | 138.076 | 1.00 | 22.32 | HIGL |
| ATOM | 117 | OE2 | GLU | 15 | 14.398 | 56.171 | 137.492 | 1.00 | 22.71 | HIGL |
| ATOM | 118 | C | GLU | 15 | 9.937 | 53.387 | 138.539 | 1.00 | 19.39 | HIGL |
| ATOM | 119 | O | GLU | 15 | 10.107 | 53.492 | 139.757 | 1.00 | 19.72 | HIGL |
| ATOM | 120 | N | GLU | 16 | 8.740 | 53.196 | 137.992 | 1.00 | 19.13 | HIGL |
| ATOM | 121 | CA | GLU | 16 | 7.562 | 53.084 | 138.839 | 1.00 | 19.39 | HIGL |
| ATOM | 122 | CB | GLU | 16 | 6.289 | 52.932 | 137.996 | 1.00 | 18.72 | HIGL |
| ATOM | 123 | CG | GLU | 16 | 5.945 | 54.180 | 137.193 | 1.00 | 19.94 | HIGL |
| ATOM | 124 | CD | GLU | 16 | 4.840 | 53.959 | 136.159 | 1.00 | 21.79 | HIGL |
| ATOM | 125 | OE1 | GLU | 16 | 4.817 | 52.881 | 135.521 | 1.00 | 22.23 | HIGL |
| ATOM | 126 | OE2 | GLU | 16 | 4.003 | 54.874 | 135.966 | 1.00 | 21.65 | HIGL |
| ATOM | 127 | C | GLU | 16 | 7.759 | 51.885 | 139.761 | 1.00 | 19.47 | HIGL |
| ATOM | 128 | O | GLU | 16 | 7.547 | 51.989 | 140.969 | 1.00 | 19.63 | HIGL |
| ATOM | 129 | N | ARG | 17 | 8.190 | 50.756 | 139.202 | 1.00 | 19.74 | HIGL |

# Fig. 2 cont.

| ATOM | 130 | CA | ARG | 17 | 8.416 | 49.562 | 140.014 | 1.00 | 20.25 | HIGL |
|------|-----|-----|-----|-----|--------|--------|---------|------|-------|------|
| ATOM | 131 | CB | ARG | 17 | 8.911 | 48.392 | 139.164 | 1.00 | 21.03 | HIGL |
| ATOM | 132 | CG | ARG | 17 | 7.873 | 47.765 | 138.257 | 1.00 | 23.68 | HIGL |
| ATOM | 133 | CD | ARG | 17 | 8.178 | 46.286 | 138.053 | 1.00 | 27.08 | HIGL |
| ATOM | 134 | NE | ARG | 17 | 7.410 | 45.701 | 136.956 | 1.00 | 31.03 | HIGL |
| ATOM | 135 | CZ | ARG | 17 | 7.660 | 45.919 | 135.664 | 1.00 | 32.87 | HIGL |
| ATOM | 136 | NH1 | ARG | 17 | 8.666 | 46.709 | 135.299 | 1.00 | 32.97 | HIGL |
| ATOM | 137 | NH2 | ARG | 17 | 6.902 | 45.352 | 134.731 | 1.00 | 33.75 | HIGL |
| ATOM | 138 | C | ARG | 17 | 9.445 | 49.840 | 141.104 | 1.00 | 19.92 | HIGL |
| ATOM | 139 | O | ARG | 17 | 9.443 | 49.198 | 142.151 | 1.00 | 20.42 | HIGL |
| ATOM | 140 | N | ALA | 18 | 10.325 | 50.801 | 140.850 | 1.00 | 19.29 | HIGL |
| ATOM | 141 | CA | ALA | 18 | 11.357 | 51.153 | 141.811 | 1.00 | 17.90 | HIGL |
| ATOM | 142 | CB | ALA | 18 | 12.584 | 51.698 | 141.086 | 1.00 | 17.12 | HIGL |
| ATOM | 143 | C | ALA | 18 | 10.846 | 52.168 | 142.830 | 1.00 | 17.59 | HIGL |
| ATOM | 144 | O | ALA | 18 | 11.611 | 52.653 | 143.669 | 1.00 | 16.93 | HIGL |
| ATOM | 145 | N | GLY | 19 | 9.557 | 52.494 | 142.745 | 1.00 | 16.98 | HIGL |
| ATOM | 146 | CA | GLY | 19 | 8.963 | 53.424 | 143.687 | 1.00 | 16.15 | HIGL |
| ATOM | 147 | C | GLY | 19 | 8.935 | 54.890 | 143.298 | 1.00 | 16.93 | HIGL |
| ATOM | 148 | O | GLY | 19 | 8.543 | 55.734 | 144.104 | 1.00 | 17.33 | HIGL |
| ATOM | 149 | N | VAL | 20 | 9.333 | 55.209 | 142.072 | 1.00 | 17.17 | HIGL |
| ATOM | 150 | CA | VAL | 20 | 9.336 | 56.598 | 141.626 | 1.00 | 17.58 | HIGL |
| ATOM | 151 | CB | VAL | 20 | 10.148 | 56.764 | 140.330 | 1.00 | 17.22 | HIGL |
| ATOM | 152 | CG1 | VAL | 20 | 10.013 | 58.190 | 139.814 | 1.00 | 16.00 | HIGL |
| ATOM | 153 | CG2 | VAL | 20 | 11.609 | 56.419 | 140.584 | 1.00 | 17.68 | HIGL |
| ATOM | 154 | C | VAL | 20 | 7.945 | 57.167 | 141.370 | 1.00 | 17.79 | HIGL |
| ATOM | 155 | O | VAL | 20 | 7.084 | 56.490 | 140.826 | 1.00 | 18.75 | HIGL |
| ATOM | 156 | N | ARG | 21 | 7.740 | 58.420 | 141.760 | 1.00 | 17.99 | HIGL |
| ATOM | 157 | CA | ARG | 21 | 6.470 | 59.106 | 141.537 | 1.00 | 18.92 | HIGL |
| ATOM | 158 | CB | ARG | 21 | 5.775 | 59.399 | 142.862 | 1.00 | 19.66 | HIGL |
| ATOM | 159 | CG | ARG | 21 | 5.367 | 58.155 | 143.617 | 1.00 | 20.84 | HIGL |
| ATOM | 160 | CD | ARG | 21 | 4.245 | 57.425 | 142.917 | 1.00 | 21.60 | HIGL |
| ATOM | 161 | NE | ARG | 21 | 3.389 | 56.783 | 143.906 | 1.00 | 23.75 | HIGL |
| ATOM | 162 | CZ | ARG | 21 | 3.734 | 55.707 | 144.598 | 1.00 | 23.89 | HIGL |
| ATOM | 163 | NH1 | ARG | 21 | 4.920 | 55.148 | 144.389 | 1.00 | 25.67 | HIGL |
| ATOM | 164 | NH2 | ARG | 21 | 2.911 | 55.215 | 145.516 | 1.00 | 22.10 | HIGL |
| ATOM | 165 | C | ARG | 21 | 6.749 | 60.412 | 140.809 | 1.00 | 18.45 | HIGL |
| ATOM | 166 | O | ARG | 21 | 7.598 | 61.198 | 141.231 | 1.00 | 18.88 | HIGL |
| ATOM | 167 | N | TYR | 22 | 6.032 | 60.640 | 139.717 | 1.00 | 17.66 | HIGL |
| ATOM | 168 | CA | TYR | 22 | 6.221 | 61.846 | 138.920 | 1.00 | 16.70 | HIGL |
| ATOM | 169 | CB | TYR | 22 | 6.236 | 61.480 | 137.438 | 1.00 | 15.81 | HIGL |
| ATOM | 170 | CG | TYR | 22 | 7.402 | 60.608 | 137.038 | 1.00 | 16.16 | HIGL |
| ATOM | 171 | CD1 | TYR | 22 | 8.706 | 61.124 | 136.998 | 1.00 | 14.69 | HIGL |
| ATOM | 172 | CE1 | TYR | 22 | 9.790 | 60.322 | 136.647 | 1.00 | 14.60 | HIGL |
| ATOM | 173 | CD2 | TYR | 22 | 7.211 | 59.260 | 136.715 | 1.00 | 15.58 | HIGL |
| ATOM | 174 | CE2 | TYR | 22 | 8.294 | 58.442 | 136.361 | 1.00 | 16.20 | HIGL |
| ATOM | 175 | CZ | TYR | 22 | 9.582 | 58.980 | 136.330 | 1.00 | 15.43 | HIGL |
| ATOM | 176 | OH | TYR | 22 | 10.648 | 58.178 | 135.994 | 1.00 | 12.55 | HIGL |
| ATOM | 177 | C | TYR | 22 | 5.156 | 62.903 | 139.166 | 1.00 | 17.06 | HIGL |
| ATOM | 178 | O | TYR | 22 | 4.008 | 62.591 | 139.482 | 1.00 | 17.73 | HIGL |
| ATOM | 179 | N | LYS | 23 | 5.545 | 64.160 | 139.011 | 1.00 | 17.11 | HIGL |
| ATOM | 180 | CA | LYS | 23 | 4.631 | 65.279 | 139.191 | 1.00 | 17.49 | HIGL |
| ATOM | 181 | CB | LYS | 23 | 4.813 | 65.913 | 140.575 | 1.00 | 18.19 | HIGL |
| ATOM | 182 | CG | LYS | 23 | 4.800 | 64.938 | 141.748 | 1.00 | 19.57 | HIGL |
| ATOM | 183 | CD | LYS | 23 | 6.141 | 64.239 | 141.933 | 1.00 | 18.82 | HIGL |
| ATOM | 184 | CE | LYS | 23 | 6.061 | 63.255 | 143.085 | 1.00 | 18.77 | HIGL |
| ATOM | 185 | NZ | LYS | 23 | 7.366 | 62.602 | 143.352 | 1.00 | 19.04 | HIGL |
| ATOM | 186 | C | LYS | 23 | 4.975 | 66.318 | 138.137 | 1.00 | 17.45 | HIGL |
| ATOM | 187 | O | LYS | 23 | 6.098 | 66.342 | 137.640 | 1.00 | 17.10 | HIGL |
| ATOM | 188 | N | ASN | 24 | 4.021 | 67.171 | 137.786 | 1.00 | 17.71 | HIGL |
| ATOM | 189 | CA | ASN | 24 | 4.315 | 68.221 | 136.823 | 1.00 | 17.61 | HIGL |
| ATOM | 190 | CB | ASN | 24 | 3.029 | 68.792 | 136.210 | 1.00 | 17.78 | HIGL |
| ATOM | 191 | CG | ASN | 24 | 1.986 | 69.174 | 137.252 | 1.00 | 17.86 | HIGL |
| ATOM | 192 | OD1 | ASN | 24 | 2.314 | 69.585 | 138.368 | 1.00 | 18.49 | HIGL |
| ATOM | 193 | ND2 | ASN | 24 | 0.717 | 69.061 | 136.876 | 1.00 | 17.05 | HIGL |
| ATOM | 194 | C | ASN | 24 | 5.081 | 69.294 | 137.597 | 1.00 | 17.97 | HIGL |

# Fig. 2 cont.

| ATOM | 195 | O | ASN | 24 | 5.481 | 69.060 | 138.739 | 1.00 | 16.84 | HIGL |
|------|-----|------|-----|----|-------|--------|---------|------|-------|------|
| ATOM | 196 | N | VAL | 25 | 5.285 | 70.462 | 136.994 | 1.00 | 19.12 | HIGL |
| ATOM | 197 | CA | VAL | 25 | 6.033 | 71.537 | 137.660 | 1.00 | 20.42 | HIGL |
| ATOM | 198 | CB | VAL | 25 | 6.164 | 72.813 | 136.789 | 1.00 | 20.47 | HIGL |
| ATOM | 199 | CG1 | VAL | 25 | 7.591 | 73.345 | 136.856 | 1.00 | 18.59 | HIGL |
| ATOM | 200 | CG2 | VAL | 25 | 5.749 | 72.534 | 135.377 | 1.00 | 21.79 | HIGL |
| ATOM | 201 | C | VAL | 25 | 5.399 | 72.009 | 138.957 | 1.00 | 20.49 | HIGL |
| ATOM | 202 | O | VAL | 25 | 6.071 | 72.577 | 139.812 | 1.00 | 19.69 | HIGL |
| ATOM | 203 | N | ASN | 26 | 4.101 | 71.782 | 139.094 | 1.00 | 21.96 | HIGL |
| ATOM | 204 | CA | ASN | 26 | 3.375 | 72.242 | 140.271 | 1.00 | 22.88 | HIGL |
| ATOM | 205 | CB | ASN | 26 | 1.979 | 72.686 | 139.841 | 1.00 | 23.37 | HIGL |
| ATOM | 206 | CG | ASN | 26 | 2.026 | 73.861 | 138.879 | 1.00 | 24.96 | HIGL |
| ATOM | 207 | OD1 | ASN | 26 | 1.188 | 73.986 | 137.980 | 1.00 | 26.06 | HIGL |
| ATOM | 208 | ND2 | ASN | 26 | 3.009 | 74.739 | 139.071 | 1.00 | 24.54 | HIGL |
| ATOM | 209 | C | ASN | 26 | 3.295 | 71.249 | 141.418 | 1.00 | 22.79 | HIGL |
| ATOM | 210 | O | ASN | 26 | 2.669 | 71.529 | 142.441 | 1.00 | 23.56 | HIGL |
| ATOM | 211 | N | GLY | 27 | 3.933 | 70.095 | 141.250 | 1.00 | 22.15 | HIGL |
| ATOM | 212 | CA | GLY | 27 | 3.932 | 69.094 | 142.299 | 1.00 | 20.67 | HIGL |
| ATOM | 213 | C | GLY | 27 | 2.743 | 68.157 | 142.290 | 1.00 | 19.93 | HIGL |
| ATOM | 214 | O | GLY | 27 | 2.574 | 67.357 | 143.214 | 1.00 | 20.18 | HIGL |
| ATOM | 215 | N | GLN | 28 | 1.912 | 68.247 | 141.258 | 1.00 | 19.35 | HIGL |
| ATOM | 216 | CA | GLN | 28 | 0.748 | 67.376 | 141.164 | 1.00 | 19.04 | HIGL |
| ATOM | 217 | CB | GLN | 28 | -0.314 | 68.025 | 140.274 | 1.00 | 19.46 | HIGL |
| ATOM | 218 | CG | GLN | 28 | -1.579 | 67.207 | 140.102 | 1.00 | 19.85 | HIGL |
| ATOM | 219 | CD | GLN | 28 | -2.666 | 67.970 | 139.363 | 1.00 | 21.15 | HIGL |
| ATOM | 220 | OE1 | GLN | 28 | -2.425 | 68.547 | 138.299 | 1.00 | 21.73 | HIGL |
| ATOM | 221 | NE2 | GLN | 28 | -3.871 | 67.971 | 139.921 | 1.00 | 20.85 | HIGL |
| ATOM | 222 | C | GLN | 28 | 1.164 | 66.009 | 140.607 | 1.00 | 18.84 | HIGL |
| ATOM | 223 | O | GLN | 28 | 1.602 | 65.901 | 139.464 | 1.00 | 18.45 | HIGL |
| ATOM | 224 | N | GLU | 29 | 1.038 | 64.973 | 141.432 | 1.00 | 18.66 | HIGL |
| ATOM | 225 | CA | GLU | 29 | 1.402 | 63.619 | 141.042 | 1.00 | 18.76 | HIGL |
| ATOM | 226 | CB | GLU | 29 | 1.487 | 62.730 | 142.287 | 1.00 | 18.41 | HIGL |
| ATOM | 227 | CG | GLU | 29 | 1.966 | 61.316 | 141.998 | 1.00 | 19.70 | HIGL |
| ATOM | 228 | CD | GLU | 29 | 2.223 | 60.504 | 143.252 | 1.00 | 21.17 | HIGL |
| ATOM | 229 | OE1 | GLU | 29 | 2.828 | 61.042 | 144.204 | 1.00 | 22.90 | HIGL |
| ATOM | 230 | OE2 | GLU | 29 | 1.836 | 59.318 | 143.285 | 1.00 | 21.00 | HIGL |
| ATOM | 231 | C | GLU | 29 | 0.412 | 63.005 | 140.045 | 1.00 | 18.74 | HIGL |
| ATOM | 232 | O | GLU | 29 | -0.793 | 63.133 | 140.205 | 1.00 | 20.35 | HIGL |
| ATOM | 233 | N | LYS | 30 | 0.929 | 62.357 | 139.007 | 1.00 | 18.03 | HIGL |
| ATOM | 234 | CA | LYS | 30 | 0.096 | 61.696 | 137.997 | 1.00 | 18.21 | HIGL |
| ATOM | 235 | CB | LYS | 30 | -0.563 | 62.702 | 137.038 | 1.00 | 18.37 | HIGL |
| ATOM | 236 | CG | LYS | 30 | -0.511 | 64.151 | 137.467 | 1.00 | 19.45 | HIGL |
| ATOM | 237 | CD | LYS | 30 | -0.017 | 65.012 | 136.323 | 1.00 | 19.01 | HIGL |
| ATOM | 238 | CE | LYS | 30 | -1.150 | 65.659 | 135.558 | 1.00 | 19.86 | HIGL |
| ATOM | 239 | NZ | LYS | 30 | -1.471 | 67.014 | 136.095 | 1.00 | 19.22 | HIGL |
| ATOM | 240 | C | LYS | 30 | 0.999 | 60.777 | 137.179 | 1.00 | 17.33 | HIGL |
| ATOM | 241 | O | LYS | 30 | 2.227 | 60.837 | 137.297 | 1.00 | 18.02 | HIGL |
| ATOM | 242 | N | PRO | 31 | 0.404 | 59.905 | 136.353 | 1.00 | 16.17 | HIGL |
| ATOM | 243 | CD | PRO | 31 | -1.032 | 59.580 | 136.274 | 1.00 | 16.56 | HIGL |
| ATOM | 244 | CA | PRO | 31 | 1.201 | 58.991 | 135.525 | 1.00 | 15.20 | HIGL |
| ATOM | 245 | CB | PRO | 31 | 0.147 | 58.122 | 134.854 | 1.00 | 15.51 | HIGL |
| ATOM | 246 | CG | PRO | 31 | -1.001 | 58.135 | 135.843 | 1.00 | 16.29 | HIGL |
| ATOM | 247 | C | PRO | 31 | 1.992 | 59.830 | 134.521 | 1.00 | 15.68 | HIGL |
| ATOM | 248 | O | PRO | 31 | 1.455 | 60.782 | 133.943 | 1.00 | 16.00 | HIGL |
| ATOM | 249 | N | LEU | 32 | 3.258 | 59.478 | 134.313 | 1.00 | 14.62 | HIGL |
| ATOM | 250 | CA | LEU | 32 | 4.139 | 60.224 | 133.416 | 1.00 | 13.57 | HIGL |
| ATOM | 251 | CB | LEU | 32 | 5.433 | 59.437 | 133.198 | 1.00 | 12.66 | HIGL |
| ATOM | 252 | CG | LEU | 32 | 6.592 | 60.142 | 132.490 | 1.00 | 12.44 | HIGL |
| ATOM | 253 | CD1 | LEU | 32 | 6.934 | 61.428 | 133.209 | 1.00 | 11.76 | HIGL |
| ATOM | 254 | CD2 | LEU | 32 | 7.805 | 59.218 | 132.455 | 1.00 | 12.43 | HIGL |
| ATOM | 255 | C | LEU | 32 | 3.546 | 60.628 | 132.062 | 1.00 | 13.85 | HIGL |
| ATOM | 256 | O | LEU | 32 | 3.684 | 61.781 | 131.641 | 1.00 | 13.20 | HIGL |
| ATOM | 257 | N | GLU | 33 | 2.881 | 59.698 | 131.379 | 1.00 | 14.00 | HIGL |
| ATOM | 258 | CA | GLU | 33 | 2.316 | 60.020 | 130.073 | 1.00 | 14.95 | HIGL |
| ATOM | 259 | CB | GLU | 33 | 1.486 | 58.847 | 129.510 | 1.00 | 15.36 | HIGL |

# Fig. 2 cont.

| ATOM | 260 | CG  | GLU | 33 | 0.259  | 58.440 | 130.324 | 1.00 | 16.87 | HIGL |
|------|-----|-----|-----|----|--------|--------|---------|------|-------|------|
| ATOM | 261 | CD  | GLU | 33 | 0.560  | 57.350 | 131.339 | 1.00 | 18.43 | HIGL |
| ATOM | 262 | OE1 | GLU | 33 | 1.586  | 57.459 | 132.049 | 1.00 | 19.77 | HIGL |
| ATOM | 263 | OE2 | GLU | 33 | -0.234 | 56.387 | 131.433 | 1.00 | 18.45 | HIGL |
| ATOM | 264 | C   | GLU | 33 | 1.476  | 61.300 | 130.102 | 1.00 | 15.90 | HIGL |
| ATOM | 265 | O   | GLU | 33 | 1.429  | 62.032 | 129.113 | 1.00 | 17.16 | HIGL |
| ATOM | 266 | N   | TYR | 34 | 0.824  | 61.584 | 131.228 | 1.00 | 16.05 | HIGL |
| ATOM | 267 | CA  | TYR | 34 | 0.005  | 62.787 | 131.325 | 1.00 | 15.44 | HIGL |
| ATOM | 268 | CB  | TYR | 34 | -1.104 | 62.593 | 132.358 | 1.00 | 16.32 | HIGL |
| ATOM | 269 | CG  | TYR | 34 | -2.087 | 61.551 | 131.901 | 1.00 | 16.99 | HIGL |
| ATOM | 270 | CD1 | TYR | 34 | -2.063 | 60.257 | 132.426 | 1.00 | 17.20 | HIGL |
| ATOM | 271 | CE1 | TYR | 34 | -2.915 | 59.267 | 131.937 | 1.00 | 17.14 | HIGL |
| ATOM | 272 | CD2 | TYR | 34 | -2.992 | 61.832 | 130.875 | 1.00 | 17.08 | HIGL |
| ATOM | 273 | CE2 | TYR | 34 | -3.845 | 60.851 | 130.378 | 1.00 | 17.17 | HIGL |
| ATOM | 274 | CZ  | TYR | 34 | -3.801 | 59.572 | 130.913 | 1.00 | 17.87 | HIGL |
| ATOM | 275 | OH  | TYR | 34 | -4.647 | 58.603 | 130.425 | 1.00 | 19.84 | HIGL |
| ATOM | 276 | C   | TYR | 34 | 0.828  | 64.030 | 131.617 | 1.00 | 14.61 | HIGL |
| ATOM | 277 | O   | TYR | 34 | 0.512  | 65.115 | 131.126 | 1.00 | 13.80 | HIGL |
| ATOM | 278 | N   | ILE | 35 | 1.889  | 63.880 | 132.399 | 1.00 | 14.26 | HIGL |
| ATOM | 279 | CA  | ILE | 35 | 2.763  | 65.014 | 132.672 | 1.00 | 14.92 | HIGL |
| ATOM | 280 | CB  | ILE | 35 | 3.865  | 64.662 | 133.679 | 1.00 | 15.08 | HIGL |
| ATOM | 281 | CG2 | ILE | 35 | 4.882  | 65.794 | 133.753 | 1.00 | 14.72 | HIGL |
| ATOM | 282 | CG1 | ILE | 35 | 3.243  | 64.398 | 135.051 | 1.00 | 15.03 | HIGL |
| ATOM | 283 | CD1 | ILE | 35 | 4.219  | 63.877 | 136.067 | 1.00 | 15.01 | HIGL |
| ATOM | 284 | C   | ILE | 35 | 3.424  | 65.404 | 131.352 | 1.00 | 14.91 | HIGL |
| ATOM | 285 | O   | ILE | 35 | 3.656  | 66.584 | 131.092 | 1.00 | 15.44 | HIGL |
| ATOM | 286 | N   | LEU | 36 | 3.715  | 64.403 | 130.518 | 1.00 | 14.83 | HIGL |
| ATOM | 287 | CA  | LEU | 36 | 4.332  | 64.649 | 129.215 | 1.00 | 14.44 | HIGL |
| ATOM | 288 | CB  | LEU | 36 | 4.765  | 63.340 | 128.557 | 1.00 | 14.34 | HIGL |
| ATOM | 289 | CG  | LEU | 36 | 5.806  | 62.491 | 129.280 | 1.00 | 15.12 | HIGL |
| ATOM | 290 | CD1 | LEU | 36 | 6.153  | 61.306 | 128.385 | 1.00 | 15.81 | HIGL |
| ATOM | 291 | CD2 | LEU | 36 | 7.050  | 63.320 | 129.595 | 1.00 | 13.46 | HIGL |
| ATOM | 292 | C   | LEU | 36 | 3.385  | 65.375 | 128.267 | 1.00 | 14.40 | HIGL |
| ATOM | 293 | O   | LEU | 36 | 3.761  | 66.376 | 127.659 | 1.00 | 13.88 | HIGL |
| ATOM | 294 | N   | ALA | 37 | 2.162  | 64.864 | 128.131 | 1.00 | 14.45 | HIGL |
| ATOM | 295 | CA  | ALA | 37 | 1.173  | 65.482 | 127.247 | 1.00 | 15.05 | HIGL |
| ATOM | 296 | CB  | ALA | 37 | -0.121 | 64.677 | 127.269 | 1.00 | 14.89 | HIGL |
| ATOM | 297 | C   | ALA | 37 | 0.918  | 66.915 | 127.711 | 1.00 | 15.47 | HIGL |
| ATOM | 298 | O   | ALA | 37 | 0.757  | 67.832 | 126.907 | 1.00 | 14.62 | HIGL |
| ATOM | 299 | N   | GLU | 38 | 0.910  | 67.081 | 129.028 | 1.00 | 16.62 | HIGL |
| ATOM | 300 | CA  | GLU | 38 | 0.693  | 68.362 | 129.689 | 1.00 | 17.33 | HIGL |
| ATOM | 301 | CB  | GLU | 38 | 0.784  | 68.145 | 131.200 | 1.00 | 19.24 | HIGL |
| ATOM | 302 | CG  | GLU | 38 | 0.365  | 69.311 | 132.054 | 1.00 | 21.29 | HIGL |
| ATOM | 303 | CD  | GLU | 38 | 0.550  | 69.028 | 133.529 | 1.00 | 22.16 | HIGL |
| ATOM | 304 | OE1 | GLU | 38 | 0.222  | 67.905 | 133.972 | 1.00 | 21.31 | HIGL |
| ATOM | 305 | OE2 | GLU | 38 | 1.018  | 69.939 | 134.244 | 1.00 | 23.91 | HIGL |
| ATOM | 306 | C   | GLU | 38 | 1.727  | 69.402 | 129.262 | 1.00 | 16.88 | HIGL |
| ATOM | 307 | O   | GLU | 38 | 1.441  | 70.597 | 129.205 | 1.00 | 16.84 | HIGL |
| ATOM | 308 | N   | ASN | 39 | 2.934  | 68.942 | 128.960 | 1.00 | 16.61 | HIGL |
| ATOM | 309 | CA  | ASN | 39 | 4.010  | 69.841 | 128.569 | 1.00 | 16.17 | HIGL |
| ATOM | 310 | CB  | ASN | 39 | 5.311  | 69.379 | 129.218 | 1.00 | 16.22 | HIGL |
| ATOM | 311 | CG  | ASN | 39 | 5.441  | 69.846 | 130.650 | 1.00 | 16.62 | HIGL |
| ATOM | 312 | OD1 | ASN | 39 | 5.928  | 70.948 | 130.907 | 1.00 | 16.26 | HIGL |
| ATOM | 313 | ND2 | ASN | 39 | 4.991  | 69.017 | 131.594 | 1.00 | 15.54 | HIGL |
| ATOM | 314 | C   | ASN | 39 | 4.218  | 70.024 | 127.067 | 1.00 | 16.04 | HIGL |
| ATOM | 315 | O   | ASN | 39 | 5.226  | 70.597 | 126.649 | 1.00 | 16.85 | HIGL |
| ATOM | 316 | N   | GLY | 40 | 3.279  | 69.535 | 126.259 | 1.00 | 15.42 | HIGL |
| ATOM | 317 | CA  | GLY | 40 | 3.392  | 69.694 | 124.821 | 1.00 | 14.77 | HIGL |
| ATOM | 318 | C   | GLY | 40 | 3.895  | 68.494 | 124.037 | 1.00 | 15.22 | HIGL |
| ATOM | 319 | O   | GLY | 40 | 3.890  | 68.517 | 122.810 | 1.00 | 15.07 | HIGL |
| ATOM | 320 | N   | VAL | 41 | 4.342  | 67.451 | 124.725 | 1.00 | 15.28 | HIGL |
| ATOM | 321 | CA  | VAL | 41 | 4.822  | 66.257 | 124.038 | 1.00 | 15.01 | HIGL |
| ATOM | 322 | CB  | VAL | 41 | 5.357  | 65.212 | 125.047 | 1.00 | 15.77 | HIGL |
| ATOM | 323 | CG1 | VAL | 41 | 5.682  | 63.896 | 124.328 | 1.00 | 14.74 | HIGL |
| ATOM | 324 | CG2 | VAL | 41 | 6.596  | 65.760 | 125.751 | 1.00 | 15.28 | HIGL |

# Fig. 2 cont.

| ATOM | 325 | C | VAL | 41 | 3.668 | 65.643 | 123.259 | 1.00 | 14.29 | HIGL |
|------|-----|-----|-----|----|-------|--------|---------|------|-------|------|
| ATOM | 326 | O | VAL | 41 | 2.560 | 65.558 | 123.776 | 1.00 | 14.34 | HIGL |
| ATOM | 327 | N | ASN | 42 | 3.913 | 65.230 | 122.017 | 1.00 | 14.20 | HIGL |
| ATOM | 328 | CA | ASN | 42 | 2.846 | 64.611 | 121.217 | 1.00 | 14.11 | HIGL |
| ATOM | 329 | CB | ASN | 42 | 2.451 | 65.488 | 120.008 | 1.00 | 13.09 | HIGL |
| ATOM | 330 | CG | ASN | 42 | 3.588 | 65.683 | 119.003 | 1.00 | 15.29 | HIGL |
| ATOM | 331 | OD1 | ASN | 42 | 4.632 | 65.030 | 119.077 | 1.00 | 14.89 | HIGL |
| ATOM | 332 | ND2 | ASN | 42 | 3.376 | 66.587 | 118.044 | 1.00 | 13.72 | HIGL |
| ATOM | 333 | C | ASN | 42 | 3.220 | 63.215 | 120.734 | 1.00 | 13.63 | HIGL |
| ATOM | 334 | O | ASN | 42 | 2.523 | 62.628 | 119.907 | 1.00 | 13.90 | HIGL |
| ATOM | 335 | N | MET | 43 | 4.319 | 62.683 | 121.259 | 1.00 | 13.09 | HIGL |
| ATOM | 336 | CA | MET | 43 | 4.776 | 61.355 | 120.865 | 1.00 | 12.43 | HIGL |
| ATOM | 337 | CB | MET | 43 | 5.290 | 61.373 | 119.421 | 1.00 | 12.54 | HIGL |
| ATOM | 338 | CG | MET | 43 | 5.833 | 60.029 | 118.943 | 1.00 | 13.16 | HIGL |
| ATOM | 339 | SD | MET | 43 | 6.153 | 59.988 | 117.164 | 1.00 | 15.39 | HIGL |
| ATOM | 340 | CE | MET | 43 | 4.461 | 60.024 | 116.523 | 1.00 | 14.86 | HIGL |
| ATOM | 341 | C | MET | 43 | 5.870 | 60.820 | 121.774 | 1.00 | 11.00 | HIGL |
| ATOM | 342 | O | MET | 43 | 6.730 | 61.563 | 122.229 | 1.00 | 9.98 | HIGL |
| ATOM | 343 | N | VAL | 44 | 5.824 | 59.522 | 122.041 | 1.00 | 10.40 | HIGL |
| ATOM | 344 | CA | VAL | 44 | 6.837 | 58.900 | 122.872 | 1.00 | 10.47 | HIGL |
| ATOM | 345 | CB | VAL | 44 | 6.218 | 58.213 | 124.113 | 1.00 | 10.16 | HIGL |
| ATOM | 346 | CG1 | VAL | 44 | 5.663 | 59.259 | 125.057 | 1.00 | 10.97 | HIGL |
| ATOM | 347 | CG2 | VAL | 44 | 5.120 | 57.251 | 123.696 | 1.00 | 10.36 | HIGL |
| ATOM | 348 | C | VAL | 44 | 7.607 | 57.868 | 122.051 | 1.00 | 10.89 | HIGL |
| ATOM | 349 | O | VAL | 44 | 7.060 | 57.241 | 121.140 | 1.00 | 9.61 | HIGL |
| ATOM | 350 | N | ARG | 45 | 8.889 | 57.721 | 122.368 | 1.00 | 11.52 | HIGL |
| ATOM | 351 | CA | ARG | 45 | 9.758 | 56.765 | 121.696 | 1.00 | 12.77 | HIGL |
| ATOM | 352 | CB | ARG | 45 | 11.085 | 57.442 | 121.351 | 1.00 | 14.01 | HIGL |
| ATOM | 353 | CG | ARG | 45 | 12.129 | 56.570 | 120.667 | 1.00 | 15.59 | HIGL |
| ATOM | 354 | CD | ARG | 45 | 13.326 | 57.430 | 120.305 | 1.00 | 16.97 | HIGL |
| ATOM | 355 | NE | ARG | 45 | 14.418 | 56.694 | 119.679 | 1.00 | 17.87 | HIGL |
| ATOM | 356 | CZ | ARG | 45 | 15.496 | 56.254 | 120.320 | 1.00 | 17.82 | HIGL |
| ATOM | 357 | NH1 | ARG | 45 | 15.642 | 56.466 | 121.620 | 1.00 | 17.90 | HIGL |
| ATOM | 358 | NH2 | ARG | 45 | 16.439 | 55.610 | 119.653 | 1.00 | 18.55 | HIGL |
| ATOM | 359 | C | ARG | 45 | 9.970 | 55.628 | 122.687 | 1.00 | 13.22 | HIGL |
| ATOM | 360 | O | ARG | 45 | 10.244 | 55.870 | 123.859 | 1.00 | 13.66 | HIGL |
| ATOM | 361 | N | GLN | 46 | 9.821 | 54.390 | 122.232 | 1.00 | 13.78 | HIGL |
| ATOM | 362 | CA | GLN | 46 | 9.996 | 53.243 | 123.118 | 1.00 | 14.54 | HIGL |
| ATOM | 363 | CB | GLN | 46 | 8.639 | 52.573 | 123.394 | 1.00 | 15.20 | HIGL |
| ATOM | 364 | CG | GLN | 46 | 7.582 | 53.492 | 124.043 | 1.00 | 16.94 | HIGL |
| ATOM | 365 | CD | GLN | 46 | 6.298 | 52.748 | 124.403 | 1.00 | 18.02 | HIGL |
| ATOM | 366 | OE1 | GLN | 46 | 5.361 | 53.328 | 124.944 | 1.00 | 17.27 | HIGL |
| ATOM | 367 | NE2 | GLN | 46 | 6.257 | 51.454 | 124.097 | 1.00 | 19.40 | HIGL |
| ATOM | 368 | C | GLN | 46 | 10.960 | 52.228 | 122.512 | 1.00 | 14.27 | HIGL |
| ATOM | 369 | O | GLN | 46 | 10.808 | 51.829 | 121.360 | 1.00 | 15.12 | HIGL |
| ATOM | 370 | N | ARG | 47 | 11.962 | 51.821 | 123.280 | 1.00 | 14.18 | HIGL |
| ATOM | 371 | CA | ARG | 47 | 12.923 | 50.847 | 122.787 | 1.00 | 14.34 | HIGL |
| ATOM | 372 | CB | ARG | 47 | 14.264 | 51.008 | 123.510 | 1.00 | 14.68 | HIGL |
| ATOM | 373 | CG | ARG | 47 | 14.172 | 51.059 | 125.026 | 1.00 | 14.19 | HIGL |
| ATOM | 374 | CD | ARG | 47 | 15.555 | 50.900 | 125.661 | 1.00 | 14.01 | HIGL |
| ATOM | 375 | NE | ARG | 47 | 15.530 | 51.133 | 127.101 | 1.00 | 13.64 | HIGL |
| ATOM | 376 | CZ | ARG | 47 | 15.463 | 52.341 | 127.651 | 1.00 | 13.65 | HIGL |
| ATOM | 377 | NH1 | ARG | 47 | 15.422 | 53.415 | 126.872 | 1.00 | 12.61 | HIGL |
| ATOM | 378 | NH2 | ARG | 47 | 15.436 | 52.479 | 128.969 | 1.00 | 12.29 | HIGL |
| ATOM | 379 | C | ARG | 47 | 12.375 | 49.434 | 122.979 | 1.00 | 14.38 | HIGL |
| ATOM | 380 | O | ARG | 47 | 11.742 | 49.139 | 123.990 | 1.00 | 14.26 | HIGL |
| ATOM | 381 | N | VAL | 48 | 12.616 | 48.567 | 121.999 | 1.00 | 14.13 | HIGL |
| ATOM | 382 | CA | VAL | 48 | 12.136 | 47.194 | 122.054 | 1.00 | 14.66 | HIGL |
| ATOM | 383 | CB | VAL | 48 | 11.108 | 46.931 | 120.946 | 1.00 | 14.30 | HIGL |
| ATOM | 384 | CG1 | VAL | 48 | 10.497 | 45.549 | 121.109 | 1.00 | 12.51 | HIGL |
| ATOM | 385 | CG2 | VAL | 48 | 10.044 | 48.001 | 120.977 | 1.00 | 14.44 | HIGL |
| ATOM | 386 | C | VAL | 48 | 13.266 | 46.185 | 121.901 | 1.00 | 15.87 | HIGL |
| ATOM | 387 | O | VAL | 48 | 13.987 | 46.200 | 120.903 | 1.00 | 16.88 | HIGL |
| ATOM | 388 | N | TRP | 49 | 13.420 | 45.319 | 122.901 | 1.00 | 16.25 | HIGL |
| ATOM | 389 | CA | TRP | 49 | 14.449 | 44.283 | 122.881 | 1.00 | 16.07 | HIGL |

# Fig. 2 cont.

| ATOM | 390 | CB  | TRP | 49 | 15.243 | 44.280 | 124.194 | 1.00 | 15.19 | HIGL |
|------|-----|-----|-----|----|--------|--------|---------|------|-------|------|
| ATOM | 391 | CG  | TRP | 49 | 16.039 | 45.533 | 124.422 | 1.00 | 15.37 | HIGL |
| ATOM | 392 | CD2 | TRP | 49 | 16.745 | 45.898 | 125.613 | 1.00 | 15.05 | HIGL |
| ATOM | 393 | CE2 | TRP | 49 | 17.359 | 47.146 | 125.370 | 1.00 | 14.69 | HIGL |
| ATOM | 394 | CE3 | TRP | 49 | 16.922 | 45.290 | 126.864 | 1.00 | 15.17 | HIGL |
| ATOM | 395 | CD1 | TRP | 49 | 16.247 | 46.550 | 123.529 | 1.00 | 15.47 | HIGL |
| ATOM | 396 | NE1 | TRP | 49 | 17.037 | 47.521 | 124.093 | 1.00 | 14.49 | HIGL |
| ATOM | 397 | CZ2 | TRP | 49 | 18.138 | 47.798 | 126.332 | 1.00 | 15.16 | HIGL |
| ATOM | 398 | CZ3 | TRP | 49 | 17.696 | 45.939 | 127.819 | 1.00 | 14.43 | HIGL |
| ATOM | 399 | CH2 | TRP | 49 | 18.294 | 47.179 | 127.547 | 1.00 | 14.14 | HIGL |
| ATOM | 400 | C   | TRP | 49 | 13.793 | 42.924 | 122.665 | 1.00 | 16.51 | HIGL |
| ATOM | 401 | O   | TRP | 49 | 12.657 | 42.695 | 123.100 | 1.00 | 16.05 | HIGL |
| ATOM | 402 | N   | VAL | 50 | 14.517 | 42.031 | 121.990 | 1.00 | 16.88 | HIGL |
| ATOM | 403 | CA  | VAL | 50 | 14.031 | 40.690 | 121.675 | 1.00 | 17.15 | HIGL |
| ATOM | 404 | CB  | VAL | 50 | 15.039 | 39.953 | 120.754 | 1.00 | 17.71 | HIGL |
| ATOM | 405 | CG1 | VAL | 50 | 14.449 | 38.639 | 120.260 | 1.00 | 17.30 | HIGL |
| ATOM | 406 | CG2 | VAL | 50 | 15.402 | 40.841 | 119.571 | 1.00 | 17.23 | HIGL |
| ATOM | 407 | C   | VAL | 50 | 13.763 | 39.843 | 122.923 | 1.00 | 17.92 | HIGL |
| ATOM | 408 | O   | VAL | 50 | 12.617 | 39.724 | 123.362 | 1.00 | 18.11 | HIGL |
| ATOM | 409 | N   | ASN | 51 | 14.812 | 39.258 | 123.495 | 1.00 | 18.58 | HIGL |
| ATOM | 410 | CA  | ASN | 51 | 14.660 | 38.430 | 124.690 | 1.00 | 18.99 | HIGL |
| ATOM | 411 | CB  | ASN | 51 | 15.126 | 37.010 | 124.410 | 1.00 | 21.64 | HIGL |
| ATOM | 412 | CG  | ASN | 51 | 14.602 | 36.480 | 123.093 | 1.00 | 24.95 | HIGL |
| ATOM | 413 | OD1 | ASN | 51 | 13.388 | 36.364 | 122.892 | 1.00 | 27.18 | HIGL |
| ATOM | 414 | ND2 | ASN | 51 | 15.517 | 36.156 | 122.180 | 1.00 | 25.56 | HIGL |
| ATOM | 415 | C   | ASN | 51 | 15.443 | 38.978 | 125.875 | 1.00 | 18.38 | HIGL |
| ATOM | 416 | O   | ASN | 51 | 16.417 | 38.368 | 126.319 | 1.00 | 17.35 | HIGL |
| ATOM | 417 | N   | PRO | 52 | 15.032 | 40.144 | 126.401 | 1.00 | 17.80 | HIGL |
| ATOM | 418 | CD  | PRO | 52 | 13.867 | 40.972 | 126.053 | 1.00 | 17.12 | HIGL |
| ATOM | 419 | CA  | PRO | 52 | 15.747 | 40.712 | 127.543 | 1.00 | 17.06 | HIGL |
| ATOM | 420 | CB  | PRO | 52 | 14.949 | 41.971 | 127.861 | 1.00 | 16.91 | HIGL |
| ATOM | 421 | CG  | PRO | 52 | 13.579 | 41.650 | 127.364 | 1.00 | 17.23 | HIGL |
| ATOM | 422 | C   | PRO | 52 | 15.776 | 39.716 | 128.688 | 1.00 | 17.60 | HIGL |
| ATOM | 423 | O   | PRO | 52 | 14.828 | 38.954 | 128.891 | 1.00 | 17.99 | HIGL |
| ATOM | 424 | N   | TRP | 53 | 16.877 | 39.723 | 129.428 | 1.00 | 17.96 | HIGL |
| ATOM | 425 | CA  | TRP | 53 | 17.068 | 38.801 | 130.536 | 1.00 | 17.77 | HIGL |
| ATOM | 426 | CB  | TRP | 53 | 18.448 | 39.013 | 131.156 | 1.00 | 18.06 | HIGL |
| ATOM | 427 | CG  | TRP | 53 | 18.543 | 40.298 | 131.917 | 1.00 | 18.50 | HIGL |
| ATOM | 428 | CD2 | TRP | 53 | 18.389 | 40.459 | 133.328 | 1.00 | 18.71 | HIGL |
| ATOM | 429 | CE2 | TRP | 53 | 18.452 | 41.844 | 133.600 | 1.00 | 17.92 | HIGL |
| ATOM | 430 | CE3 | TRP | 53 | 18.198 | 39.565 | 134.390 | 1.00 | 18.46 | HIGL |
| ATOM | 431 | CD1 | TRP | 53 | 18.698 | 41.553 | 131.404 | 1.00 | 18.32 | HIGL |
| ATOM | 432 | NE1 | TRP | 53 | 18.642 | 42.489 | 132.409 | 1.00 | 17.61 | HIGL |
| ATOM | 433 | CZ2 | TRP | 53 | 18.331 | 42.357 | 134.888 | 1.00 | 19.23 | HIGL |
| ATOM | 434 | CZ3 | TRP | 53 | 18.077 | 40.074 | 135.674 | 1.00 | 19.45 | HIGL |
| ATOM | 435 | CH2 | TRP | 53 | 18.143 | 41.460 | 135.912 | 1.00 | 19.83 | HIGL |
| ATOM | 436 | C   | TRP | 53 | 16.017 | 38.919 | 131.631 | 1.00 | 17.78 | HIGL |
| ATOM | 437 | O   | TRP | 53 | 15.726 | 37.944 | 132.324 | 1.00 | 18.33 | HIGL |
| ATOM | 438 | N   | ASP | 54 | 15.447 | 40.106 | 131.793 | 1.00 | 17.42 | HIGL |
| ATOM | 439 | CA  | ASP | 54 | 14.455 | 40.307 | 132.845 | 1.00 | 17.12 | HIGL |
| ATOM | 440 | CB  | ASP | 54 | 14.976 | 41.352 | 133.830 | 1.00 | 16.85 | HIGL |
| ATOM | 441 | CG  | ASP | 54 | 15.139 | 42.705 | 133.189 | 1.00 | 17.98 | HIGL |
| ATOM | 442 | OD1 | ASP | 54 | 15.083 | 42.779 | 131.938 | 1.00 | 19.62 | HIGL |
| ATOM | 443 | OD2 | ASP | 54 | 15.325 | 43.690 | 133.927 | 1.00 | 17.75 | HIGL |
| ATOM | 444 | C   | ASP | 54 | 13.080 | 40.718 | 132.320 | 1.00 | 16.46 | HIGL |
| ATOM | 445 | O   | ASP | 54 | 12.196 | 41.080 | 133.094 | 1.00 | 16.77 | HIGL |
| ATOM | 446 | N   | GLY | 55 | 12.907 | 40.666 | 131.003 | 1.00 | 16.49 | HIGL |
| ATOM | 447 | CA  | GLY | 55 | 11.629 | 41.019 | 130.406 | 1.00 | 15.10 | HIGL |
| ATOM | 448 | C   | GLY | 55 | 11.396 | 42.494 | 130.120 | 1.00 | 14.82 | HIGL |
| ATOM | 449 | O   | GLY | 55 | 10.461 | 42.844 | 129.401 | 1.00 | 14.82 | HIGL |
| ATOM | 450 | N   | ASN | 56 | 12.225 | 43.375 | 130.667 | 1.00 | 14.46 | HIGL |
| ATOM | 451 | CA  | ASN | 56 | 12.010 | 44.792 | 130.418 | 1.00 | 14.01 | HIGL |
| ATOM | 452 | CB  | ASN | 56 | 12.784 | 45.649 | 131.417 | 1.00 | 14.38 | HIGL |
| ATOM | 453 | CG  | ASN | 56 | 12.130 | 45.660 | 132.785 | 1.00 | 15.79 | HIGL |
| ATOM | 454 | OD1 | ASN | 56 | 10.901 | 45.606 | 132.902 | 1.00 | 15.70 | HIGL |

# Fig. 2 cont.

| ATOM | 455 | ND2 | ASN | 56 | 12.941 | 45.743 | 133.826 | 1.00 | 16.95 | HIGL |
|------|-----|-----|-----|----|--------|--------|---------|------|-------|------|
| ATOM | 456 | C | ASN | 56 | 12.341 | 45.204 | 128.999 | 1.00 | 13.31 | HIGL |
| ATOM | 457 | O | ASN | 56 | 13.366 | 44.817 | 128.442 | 1.00 | 12.12 | HIGL |
| ATOM | 458 | N | TYR | 57 | 11.439 | 45.991 | 128.424 | 1.00 | 13.34 | HIGL |
| ATOM | 459 | CA | TYR | 57 | 11.558 | 46.499 | 127.065 | 1.00 | 13.09 | HIGL |
| ATOM | 460 | CB | TYR | 57 | 12.968 | 47.049 | 126.789 | 1.00 | 12.20 | HIGL |
| ATOM | 461 | CG | TYR | 57 | 13.466 | 47.989 | 127.865 | 1.00 | 11.14 | HIGL |
| ATOM | 462 | CD1 | TYR | 57 | 12.666 | 49.030 | 128.330 | 1.00 | 10.28 | HIGL |
| ATOM | 463 | CE1 | TYR | 57 | 13.095 | 49.859 | 129.353 | 1.00 | 9.79 | HIGL |
| ATOM | 464 | CD2 | TYR | 57 | 14.716 | 47.808 | 128.450 | 1.00 | 10.12 | HIGL |
| ATOM | 465 | CE2 | TYR | 57 | 15.152 | 48.630 | 129.471 | 1.00 | 9.28 | HIGL |
| ATOM | 466 | CZ | TYR | 57 | 14.333 | 49.654 | 129.922 | 1.00 | 9.42 | HIGL |
| ATOM | 467 | OH | TYR | 57 | 14.737 | 50.450 | 130.973 | 1.00 | 10.17 | HIGL |
| ATOM | 468 | C | TYR | 57 | 11.214 | 45.426 | 126.052 | 1.00 | 13.71 | HIGL |
| ATOM | 469 | O | TYR | 57 | 11.460 | 45.591 | 124.854 | 1.00 | 13.96 | HIGL |
| ATOM | 470 | N | ASN | 58 | 10.657 | 44.313 | 126.515 | 1.00 | 13.75 | HIGL |
| ATOM | 471 | CA | ASN | 58 | 10.276 | 43.298 | 125.553 | 1.00 | 14.27 | HIGL |
| ATOM | 472 | CB | ASN | 58 | 10.325 | 41.874 | 126.147 | 1.00 | 12.09 | HIGL |
| ATOM | 473 | CG | ASN | 58 | 9.216 | 41.576 | 127.140 | 1.00 | 9.87 | HIGL |
| ATOM | 474 | OD1 | ASN | 58 | 8.278 | 42.353 | 127.323 | 1.00 | 11.38 | HIGL |
| ATOM | 475 | ND2 | ASN | 58 | 9.316 | 40.416 | 127.777 | 1.00 | 5.89 | HIGL |
| ATOM | 476 | C | ASN | 58 | 8.892 | 43.669 | 125.039 | 1.00 | 15.29 | HIGL |
| ATOM | 477 | O | ASN | 58 | 8.301 | 44.651 | 125.490 | 1.00 | 14.81 | HIGL |
| ATOM | 478 | N | LEU | 59 | 8.389 | 42.901 | 124.085 | 1.00 | 17.30 | HIGL |
| ATOM | 479 | CA | LEU | 59 | 7.096 | 43.188 | 123.482 | 1.00 | 19.48 | HIGL |
| ATOM | 480 | CB | LEU | 59 | 6.692 | 42.037 | 122.565 | 1.00 | 21.08 | HIGL |
| ATOM | 481 | CG | LEU | 59 | 5.709 | 42.447 | 121.470 | 1.00 | 23.34 | HIGL |
| ATOM | 482 | CD1 | LEU | 59 | 6.296 | 43.624 | 120.673 | 1.00 | 23.05 | HIGL |
| ATOM | 483 | CD2 | LEU | 59 | 5.436 | 41.247 | 120.561 | 1.00 | 23.47 | HIGL |
| ATOM | 484 | C | LEU | 59 | 5.970 | 43.488 | 124.471 | 1.00 | 19.90 | HIGL |
| ATOM | 485 | O | LEU | 59 | 5.367 | 44.557 | 124.415 | 1.00 | 21.04 | HIGL |
| ATOM | 486 | N | ASP | 60 | 5.683 | 42.555 | 125.372 | 1.00 | 20.10 | HIGL |
| ATOM | 487 | CA | ASP | 60 | 4.619 | 42.756 | 126.348 | 1.00 | 20.50 | HIGL |
| ATOM | 488 | CB | ASP | 60 | 4.599 | 41.613 | 127.369 | 1.00 | 21.74 | HIGL |
| ATOM | 489 | CG | ASP | 60 | 4.436 | 40.250 | 126.720 | 1.00 | 23.55 | HIGL |
| ATOM | 490 | OD1 | ASP | 60 | 3.553 | 40.100 | 125.844 | 1.00 | 23.00 | HIGL |
| ATOM | 491 | OD2 | ASP | 60 | 5.190 | 39.324 | 127.094 | 1.00 | 24.89 | HIGL |
| ATOM | 492 | C | ASP | 60 | 4.810 | 44.078 | 127.078 | 1.00 | 20.77 | HIGL |
| ATOM | 493 | O | ASP | 60 | 3.869 | 44.860 | 127.231 | 1.00 | 21.37 | HIGL |
| ATOM | 494 | N | TYR | 61 | 6.038 | 44.315 | 127.529 | 1.00 | 20.29 | HIGL |
| ATOM | 495 | CA | TYR | 61 | 6.393 | 45.533 | 128.241 | 1.00 | 19.19 | HIGL |
| ATOM | 496 | CB | TYR | 61 | 7.896 | 45.526 | 128.574 | 1.00 | 19.77 | HIGL |
| ATOM | 497 | CG | TYR | 61 | 8.400 | 46.776 | 129.274 | 1.00 | 19.20 | HIGL |
| ATOM | 498 | CD1 | TYR | 61 | 8.572 | 47.975 | 128.580 | 1.00 | 19.12 | HIGL |
| ATOM | 499 | CE1 | TYR | 61 | 8.998 | 49.132 | 129.229 | 1.00 | 19.60 | HIGL |
| ATOM | 500 | CD2 | TYR | 61 | 8.675 | 46.766 | 130.638 | 1.00 | 19.18 | HIGL |
| ATOM | 501 | CE2 | TYR | 61 | 9.101 | 47.916 | 131.297 | 1.00 | 20.13 | HIGL |
| ATOM | 502 | CZ | TYR | 61 | 9.259 | 49.096 | 130.589 | 1.00 | 20.45 | HIGL |
| ATOM | 503 | OH | TYR | 61 | 9.663 | 50.239 | 131.250 | 1.00 | 21.00 | HIGL |
| ATOM | 504 | C | TYR | 61 | 6.059 | 46.767 | 127.414 | 1.00 | 19.25 | HIGL |
| ATOM | 505 | O | TYR | 61 | 5.506 | 47.738 | 127.930 | 1.00 | 19.40 | HIGL |
| ATOM | 506 | N | ASN | 62 | 6.390 | 46.733 | 126.129 | 1.00 | 19.00 | HIGL |
| ATOM | 507 | CA | ASN | 62 | 6.128 | 47.878 | 125.271 | 1.00 | 19.77 | HIGL |
| ATOM | 508 | CB | ASN | 62 | 6.971 | 47.789 | 123.999 | 1.00 | 20.44 | HIGL |
| ATOM | 509 | CG | ASN | 62 | 8.403 | 48.223 | 124.229 | 1.00 | 21.08 | HIGL |
| ATOM | 510 | OD1 | ASN | 62 | 8.685 | 49.415 | 124.376 | 1.00 | 21.94 | HIGL |
| ATOM | 511 | ND2 | ASN | 62 | 9.315 | 47.259 | 124.284 | 1.00 | 20.37 | HIGL |
| ATOM | 512 | C | ASN | 62 | 4.664 | 48.053 | 124.925 | 1.00 | 19.75 | HIGL |
| ATOM | 513 | O | ASN | 62 | 4.235 | 49.156 | 124.588 | 1.00 | 20.46 | HIGL |
| ATOM | 514 | N | ILE | 63 | 3.892 | 46.977 | 125.009 | 1.00 | 19.62 | HIGL |
| ATOM | 515 | CA | ILE | 63 | 2.472 | 47.073 | 124.717 | 1.00 | 20.26 | HIGL |
| ATOM | 516 | CB | ILE | 63 | 1.856 | 45.693 | 124.478 | 1.00 | 20.11 | HIGL |
| ATOM | 517 | CG2 | ILE | 63 | 0.336 | 45.761 | 124.598 | 1.00 | 19.41 | HIGL |
| ATOM | 518 | CG1 | ILE | 63 | 2.293 | 45.198 | 123.101 | 1.00 | 20.67 | HIGL |
| ATOM | 519 | CD1 | ILE | 63 | 1.599 | 43.952 | 122.648 | 1.00 | 23.84 | HIGL |

# Fig. 2 cont.

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| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 520 | C | ILE | 63 | 1.742 | 47.775 | 125.852 | 1.00 | 21.15 | HIGL |
| ATOM | 521 | O | ILE | 63 | 0.807 | 48.535 | 125.617 | 1.00 | 20.59 | HIGL |
| ATOM | 522 | N | GLN | 64 | 2.172 | 47.528 | 127.086 | 1.00 | 22.72 | HIGL |
| ATOM | 523 | CA | GLN | 64 | 1.547 | 48.177 | 128.235 | 1.00 | 23.28 | HIGL |
| ATOM | 524 | CB | GLN | 64 | 2.117 | 47.626 | 129.544 | 1.00 | 24.62 | HIGL |
| ATOM | 525 | CG | GLN | 64 | 1.064 | 47.428 | 130.630 | 1.00 | 27.22 | HIGL |
| ATOM | 526 | CD | GLN | 64 | 1.641 | 46.837 | 131.906 | 1.00 | 29.98 | HIGL |
| ATOM | 527 | OE1 | GLN | 64 | 2.314 | 45.798 | 131.877 | 1.00 | 31.39 | HIGL |
| ATOM | 528 | NE2 | GLN | 64 | 1.380 | 47.493 | 133.037 | 1.00 | 29.60 | HIGL |
| ATOM | 529 | C | GLN | 64 | 1.827 | 49.675 | 128.130 | 1.00 | 22.91 | HIGL |
| ATOM | 530 | O | GLN | 64 | 0.952 | 50.501 | 128.400 | 1.00 | 23.24 | HIGL |
| ATOM | 531 | N | LEU | 65 | 3.045 | 50.018 | 127.717 | 1.00 | 21.90 | HIGL |
| ATOM | 532 | CA | LEU | 65 | 3.436 | 51.415 | 127.559 | 1.00 | 21.80 | HIGL |
| ATOM | 533 | CB | LEU | 65 | 4.925 | 51.524 | 127.241 | 1.00 | 21.78 | HIGL |
| ATOM | 534 | CG | LEU | 65 | 5.863 | 51.436 | 128.439 | 1.00 | 22.02 | HIGL |
| ATOM | 535 | CD1 | LEU | 65 | 7.300 | 51.702 | 128.006 | 1.00 | 21.72 | HIGL |
| ATOM | 536 | CD2 | LEU | 65 | 5.424 | 52.459 | 129.459 | 1.00 | 22.32 | HIGL |
| ATOM | 537 | C | LEU | 65 | 2.650 | 52.104 | 126.458 | 1.00 | 21.48 | HIGL |
| ATOM | 538 | O | LEU | 65 | 2.107 | 53.191 | 126.651 | 1.00 | 20.27 | HIGL |
| ATOM | 539 | N | ALA | 66 | 2.604 | 51.467 | 125.297 | 1.00 | 21.88 | HIGL |
| ATOM | 540 | CA | ALA | 66 | 1.884 | 52.017 | 124.157 | 1.00 | 22.71 | HIGL |
| ATOM | 541 | CB | ALA | 66 | 1.908 | 51.026 | 123.006 | 1.00 | 21.67 | HIGL |
| ATOM | 542 | C | ALA | 66 | 0.447 | 52.340 | 124.546 | 1.00 | 22.91 | HIGL |
| ATOM | 543 | O | ALA | 66 | −0.013 | 53.471 | 124.395 | 1.00 | 23.72 | HIGL |
| ATOM | 544 | N | ARG | 67 | −0.256 | 51.340 | 125.059 | 1.00 | 23.00 | HIGL |
| ATOM | 545 | CA | ARG | 67 | −1.635 | 51.517 | 125.457 | 1.00 | 22.83 | HIGL |
| ATOM | 546 | CB | ARG | 67 | −2.121 | 50.260 | 126.173 | 1.00 | 24.13 | HIGL |
| ATOM | 547 | CG | ARG | 67 | −3.621 | 50.147 | 126.305 | 1.00 | 26.38 | HIGL |
| ATOM | 548 | CD | ARG | 67 | −3.993 | 48.774 | 126.824 | 1.00 | 29.10 | HIGL |
| ATOM | 549 | NE | ARG | 67 | −3.810 | 47.732 | 125.815 | 1.00 | 30.83 | HIGL |
| ATOM | 550 | CZ | ARG | 67 | −3.501 | 46.469 | 126.098 | 1.00 | 32.31 | HIGL |
| ATOM | 551 | NH1 | ARG | 67 | −3.333 | 46.096 | 127.361 | 1.00 | 33.65 | HIGL |
| ATOM | 552 | NH2 | ARG | 67 | −3.369 | 45.576 | 125.126 | 1.00 | 32.30 | HIGL |
| ATOM | 553 | C | ARG | 67 | −1.747 | 52.749 | 126.351 | 1.00 | 22.02 | HIGL |
| ATOM | 554 | O | ARG | 67 | −2.627 | 53.587 | 126.158 | 1.00 | 22.49 | HIGL |
| ATOM | 555 | N | ARG | 68 | −0.843 | 52.876 | 127.313 | 1.00 | 21.00 | HIGL |
| ATOM | 556 | CA | ARG | 68 | −0.860 | 54.031 | 128.207 | 1.00 | 20.10 | HIGL |
| ATOM | 557 | CB | ARG | 68 | 0.183 | 53.867 | 129.321 | 1.00 | 19.58 | HIGL |
| ATOM | 558 | CG | ARG | 68 | −0.247 | 52.927 | 130.442 | 1.00 | 18.60 | HIGL |
| ATOM | 559 | CD | ARG | 68 | 0.858 | 52.723 | 131.475 | 1.00 | 17.98 | HIGL |
| ATOM | 560 | NE | ARG | 68 | 1.319 | 53.986 | 132.048 | 1.00 | 17.78 | HIGL |
| ATOM | 561 | CZ | ARG | 68 | 2.210 | 54.078 | 133.030 | 1.00 | 16.65 | HIGL |
| ATOM | 562 | NH1 | ARG | 68 | 2.735 | 52.975 | 133.550 | 1.00 | 15.08 | HIGL |
| ATOM | 563 | NH2 | ARG | 68 | 2.574 | 55.272 | 133.490 | 1.00 | 15.87 | HIGL |
| ATOM | 564 | C | ARG | 68 | −0.588 | 55.322 | 127.441 | 1.00 | 20.06 | HIGL |
| ATOM | 565 | O | ARG | 68 | −1.287 | 56.312 | 127.613 | 1.00 | 19.99 | HIGL |
| ATOM | 566 | N | ALA | 69 | 0.437 | 55.306 | 126.597 | 1.00 | 20.75 | HIGL |
| ATOM | 567 | CA | ALA | 69 | 0.800 | 56.477 | 125.808 | 1.00 | 21.00 | HIGL |
| ATOM | 568 | CB | ALA | 69 | 1.979 | 56.144 | 124.913 | 1.00 | 21.37 | HIGL |
| ATOM | 569 | C | ALA | 69 | −0.379 | 56.960 | 124.965 | 1.00 | 21.40 | HIGL |
| ATOM | 570 | O | ALA | 69 | −0.610 | 58.164 | 124.829 | 1.00 | 20.93 | HIGL |
| ATOM | 571 | N | LYS | 70 | −1.114 | 56.007 | 124.402 | 1.00 | 21.23 | HIGL |
| ATOM | 572 | CA | LYS | 70 | −2.273 | 56.295 | 123.574 | 1.00 | 22.04 | HIGL |
| ATOM | 573 | CB | LYS | 70 | −2.770 | 54.991 | 122.941 | 1.00 | 24.06 | HIGL |
| ATOM | 574 | CG | LYS | 70 | −4.006 | 55.118 | 122.060 | 1.00 | 26.72 | HIGL |
| ATOM | 575 | CD | LYS | 70 | −4.553 | 53.734 | 121.710 | 1.00 | 29.26 | HIGL |
| ATOM | 576 | CE | LYS | 70 | −5.785 | 53.811 | 120.813 | 1.00 | 30.47 | HIGL |
| ATOM | 577 | NZ | LYS | 70 | −6.349 | 52.451 | 120.547 | 1.00 | 31.87 | HIGL |
| ATOM | 578 | C | LYS | 70 | −3.394 | 56.946 | 124.403 | 1.00 | 21.81 | HIGL |
| ATOM | 579 | O | LYS | 70 | −4.034 | 57.901 | 123.958 | 1.00 | 21.40 | HIGL |
| ATOM | 580 | N | ALA | 71 | −3.631 | 56.439 | 125.609 | 1.00 | 20.36 | HIGL |
| ATOM | 581 | CA | ALA | 71 | −4.682 | 57.000 | 126.448 | 1.00 | 19.90 | HIGL |
| ATOM | 582 | CB | ALA | 71 | −4.770 | 56.242 | 127.767 | 1.00 | 19.16 | HIGL |
| ATOM | 583 | C | ALA | 71 | −4.432 | 58.485 | 126.708 | 1.00 | 19.54 | HIGL |
| ATOM | 584 | O | ALA | 71 | −5.371 | 59.259 | 126.862 | 1.00 | 20.19 | HIGL |

# Fig. 2 cont.

| ATOM | 585 | N   | ALA | 72 | -3.166 | 58.881 | 126.754 | 1.00 | 18.45 | HIGL |
| ATOM | 586 | CA  | ALA | 72 | -2.822 | 60.276 | 126.987 | 1.00 | 17.24 | HIGL |
| ATOM | 587 | CB  | ALA | 72 | -1.507 | 60.374 | 127.753 | 1.00 | 16.31 | HIGL |
| ATOM | 588 | C   | ALA | 72 | -2.722 | 61.035 | 125.667 | 1.00 | 16.70 | HIGL |
| ATOM | 589 | O   | ALA | 72 | -2.210 | 62.147 | 125.628 | 1.00 | 17.88 | HIGL |
| ATOM | 590 | N   | GLY | 73 | -3.200 | 60.421 | 124.589 | 1.00 | 15.95 | HIGL |
| ATOM | 591 | CA  | GLY | 73 | -3.176 | 61.058 | 123.284 | 1.00 | 15.41 | HIGL |
| ATOM | 592 | C   | GLY | 73 | -1.809 | 61.236 | 122.647 | 1.00 | 16.92 | HIGL |
| ATOM | 593 | O   | GLY | 73 | -1.638 | 62.056 | 121.739 | 1.00 | 16.80 | HIGL |
| ATOM | 594 | N   | LEU | 74 | -0.826 | 60.470 | 123.107 | 1.00 | 16.80 | HIGL |
| ATOM | 595 | CA  | LEU | 74 | 0.516 | 60.577 | 122.554 | 1.00 | 16.41 | HIGL |
| ATOM | 596 | CB  | LEU | 74 | 1.545 | 60.366 | 123.663 | 1.00 | 15.23 | HIGL |
| ATOM | 597 | CG  | LEU | 74 | 1.311 | 61.253 | 124.884 | 1.00 | 14.82 | HIGL |
| ATOM | 598 | CD1 | LEU | 74 | 2.265 | 60.875 | 125.994 | 1.00 | 13.72 | HIGL |
| ATOM | 599 | CD2 | LEU | 74 | 1.486 | 62.706 | 124.492 | 1.00 | 14.41 | HIGL |
| ATOM | 600 | C   | LEU | 74 | 0.762 | 59.577 | 121.424 | 1.00 | 17.36 | HIGL |
| ATOM | 601 | O   | LEU | 74 | 0.319 | 58.430 | 121.482 | 1.00 | 16.67 | HIGL |
| ATOM | 602 | N   | GLY | 75 | 1.470 | 60.027 | 120.392 | 1.00 | 18.17 | HIGL |
| ATOM | 603 | CA  | GLY | 75 | 1.785 | 59.155 | 119.278 | 1.00 | 17.81 | HIGL |
| ATOM | 604 | C   | GLY | 75 | 2.846 | 58.153 | 119.695 | 1.00 | 18.44 | HIGL |
| ATOM | 605 | O   | GLY | 75 | 3.486 | 58.299 | 120.748 | 1.00 | 18.86 | HIGL |
| ATOM | 606 | N   | LEU | 76 | 3.058 | 57.147 | 118.858 | 1.00 | 17.36 | HIGL |
| ATOM | 607 | CA  | LEU | 76 | 4.014 | 56.103 | 119.163 | 1.00 | 16.84 | HIGL |
| ATOM | 608 | CB  | LEU | 76 | 3.262 | 54.777 | 119.306 | 1.00 | 16.53 | HIGL |
| ATOM | 609 | CG  | LEU | 76 | 4.075 | 53.527 | 119.631 | 1.00 | 17.06 | HIGL |
| ATOM | 610 | CD1 | LEU | 76 | 4.742 | 53.691 | 120.997 | 1.00 | 16.56 | HIGL |
| ATOM | 611 | CD2 | LEU | 76 | 3.161 | 52.318 | 119.620 | 1.00 | 15.85 | HIGL |
| ATOM | 612 | C   | LEU | 76 | 5.143 | 55.949 | 118.139 | 1.00 | 16.79 | HIGL |
| ATOM | 613 | O   | LEU | 76 | 4.914 | 55.918 | 116.932 | 1.00 | 17.69 | HIGL |
| ATOM | 614 | N   | TYR | 77 | 6.364 | 55.844 | 118.648 | 1.00 | 15.89 | HIGL |
| ATOM | 615 | CA  | TYR | 77 | 7.560 | 55.664 | 117.835 | 1.00 | 15.08 | HIGL |
| ATOM | 616 | CB  | TYR | 77 | 8.420 | 56.938 | 117.927 | 1.00 | 14.34 | HIGL |
| ATOM | 617 | CG  | TYR | 77 | 9.866 | 56.872 | 117.435 | 1.00 | 14.79 | HIGL |
| ATOM | 618 | CD1 | TYR | 77 | 10.428 | 55.695 | 116.925 | 1.00 | 13.89 | HIGL |
| ATOM | 619 | CE1 | TYR | 77 | 11.774 | 55.644 | 116.552 | 1.00 | 14.56 | HIGL |
| ATOM | 620 | CD2 | TYR | 77 | 10.693 | 57.994 | 117.547 | 1.00 | 15.32 | HIGL |
| ATOM | 621 | CE2 | TYR | 77 | 12.039 | 57.955 | 117.179 | 1.00 | 14.67 | HIGL |
| ATOM | 622 | CZ  | TYR | 77 | 12.577 | 56.783 | 116.688 | 1.00 | 15.26 | HIGL |
| ATOM | 623 | OH  | TYR | 77 | 13.920 | 56.753 | 116.367 | 1.00 | 14.00 | HIGL |
| ATOM | 624 | C   | TYR | 77 | 8.261 | 54.436 | 118.440 | 1.00 | 15.55 | HIGL |
| ATOM | 625 | O   | TYR | 77 | 8.853 | 54.507 | 119.530 | 1.00 | 15.30 | HIGL |
| ATOM | 626 | N   | ILE | 78 | 8.147 | 53.306 | 117.743 | 1.00 | 14.24 | HIGL |
| ATOM | 627 | CA  | ILE | 78 | 8.751 | 52.051 | 118.183 | 1.00 | 14.13 | HIGL |
| ATOM | 628 | CB  | ILE | 78 | 7.970 | 50.824 | 117.639 | 1.00 | 14.46 | HIGL |
| ATOM | 629 | CG2 | ILE | 78 | 8.742 | 49.534 | 117.930 | 1.00 | 14.89 | HIGL |
| ATOM | 630 | CG1 | ILE | 78 | 6.575 | 50.766 | 118.276 | 1.00 | 14.25 | HIGL |
| ATOM | 631 | CD1 | ILE | 78 | 6.567 | 50.420 | 119.761 | 1.00 | 12.73 | HIGL |
| ATOM | 632 | C   | ILE | 78 | 10.193 | 51.991 | 117.701 | 1.00 | 13.40 | HIGL |
| ATOM | 633 | O   | ILE | 78 | 10.467 | 52.112 | 116.512 | 1.00 | 13.27 | HIGL |
| ATOM | 634 | N   | ASN | 79 | 11.104 | 51.797 | 118.646 | 1.00 | 13.08 | HIGL |
| ATOM | 635 | CA  | ASN | 79 | 12.533 | 51.753 | 118.378 | 1.00 | 12.27 | HIGL |
| ATOM | 636 | CB  | ASN | 79 | 13.209 | 52.771 | 119.304 | 1.00 | 12.87 | HIGL |
| ATOM | 637 | CG  | ASN | 79 | 14.714 | 52.607 | 119.393 | 1.00 | 12.44 | HIGL |
| ATOM | 638 | OD1 | ASN | 79 | 15.291 | 52.886 | 120.435 | 1.00 | 12.93 | HIGL |
| ATOM | 639 | ND2 | ASN | 79 | 15.353 | 52.175 | 118.311 | 1.00 | 12.14 | HIGL |
| ATOM | 640 | C   | ASN | 79 | 13.111 | 50.354 | 118.587 | 1.00 | 12.54 | HIGL |
| ATOM | 641 | O   | ASN | 79 | 13.453 | 49.979 | 119.708 | 1.00 | 12.54 | HIGL |
| ATOM | 642 | N   | PHE | 80 | 13.209 | 49.590 | 117.501 | 1.00 | 12.76 | HIGL |
| ATOM | 643 | CA  | PHE | 80 | 13.752 | 48.232 | 117.534 | 1.00 | 13.01 | HIGL |
| ATOM | 644 | CB  | PHE | 80 | 13.453 | 47.486 | 116.228 | 1.00 | 12.75 | HIGL |
| ATOM | 645 | CG  | PHE | 80 | 12.076 | 46.901 | 116.154 | 1.00 | 13.87 | HIGL |
| ATOM | 646 | CD1 | PHE | 80 | 11.636 | 45.998 | 117.120 | 1.00 | 13.28 | HIGL |
| ATOM | 647 | CD2 | PHE | 80 | 11.218 | 47.241 | 115.114 | 1.00 | 12.89 | HIGL |
| ATOM | 648 | CE1 | PHE | 80 | 10.363 | 45.446 | 117.054 | 1.00 | 11.74 | HIGL |
| ATOM | 649 | CE2 | PHE | 80 | 9.943 | 46.692 | 115.043 | 1.00 | 13.92 | HIGL |

# Fig. 2 cont.

| ATOM | 650 | CZ | PHE | 80 | 9.517 | 45.792 | 116.019 | 1.00 | 13.02 | HIGL |
|------|-----|-----|-----|-----|--------|--------|---------|------|-------|------|
| ATOM | 651 | C | PHE | 80 | 15.259 | 48.253 | 117.690 | 1.00 | 13.33 | HIGL |
| ATOM | 652 | O | PHE | 80 | 15.937 | 48.944 | 116.940 | 1.00 | 14.29 | HIGL |
| ATOM | 653 | N | HIS | 81 | 15.784 | 47.499 | 118.649 | 1.00 | 12.98 | HIGL |
| ATOM | 654 | CA | HIS | 81 | 17.227 | 47.426 | 118.823 | 1.00 | 13.87 | HIGL |
| ATOM | 655 | CB | HIS | 81 | 17.626 | 47.425 | 120.304 | 1.00 | 13.89 | HIGL |
| ATOM | 656 | CG | HIS | 81 | 17.633 | 48.782 | 120.933 | 1.00 | 15.21 | HIGL |
| ATOM | 657 | CD2 | HIS | 81 | 16.749 | 49.805 | 120.860 | 1.00 | 15.13 | HIGL |
| ATOM | 658 | ND1 | HIS | 81 | 18.639 | 49.204 | 121.777 | 1.00 | 15.56 | HIGL |
| ATOM | 659 | CE1 | HIS | 81 | 18.375 | 50.429 | 122.196 | 1.00 | 14.49 | HIGL |
| ATOM | 660 | NE2 | HIS | 81 | 17.234 | 50.816 | 121.655 | 1.00 | 15.27 | HIGL |
| ATOM | 661 | C | HIS | 81 | 17.717 | 46.137 | 118.176 | 1.00 | 13.69 | HIGL |
| ATOM | 662 | O | HIS | 81 | 18.911 | 45.971 | 117.928 | 1.00 | 14.21 | HIGL |
| ATOM | 663 | N | TYR | 82 | 16.784 | 45.231 | 117.902 | 1.00 | 13.26 | HIGL |
| ATOM | 664 | CA | TYR | 82 | 17.105 | 43.939 | 117.299 | 1.00 | 13.09 | HIGL |
| ATOM | 665 | CB | TYR | 82 | 17.449 | 44.102 | 115.819 | 1.00 | 13.22 | HIGL |
| ATOM | 666 | CG | TYR | 82 | 16.277 | 44.556 | 114.986 | 1.00 | 13.70 | HIGL |
| ATOM | 667 | CD1 | TYR | 82 | 15.014 | 43.977 | 115.161 | 1.00 | 13.38 | HIGL |
| ATOM | 668 | CE1 | TYR | 82 | 13.939 | 44.348 | 114.378 | 1.00 | 12.96 | HIGL |
| ATOM | 669 | CD2 | TYR | 82 | 16.429 | 45.529 | 114.002 | 1.00 | 12.39 | HIGL |
| ATOM | 670 | CE2 | TYR | 82 | 15.359 | 45.908 | 113.209 | 1.00 | 13.19 | HIGL |
| ATOM | 671 | CZ | TYR | 82 | 14.114 | 45.310 | 113.400 | 1.00 | 14.02 | HIGL |
| ATOM | 672 | OH | TYR | 82 | 13.046 | 45.652 | 112.595 | 1.00 | 15.86 | HIGL |
| ATOM | 673 | C | TYR | 82 | 18.257 | 43.278 | 118.030 | 1.00 | 13.08 | HIGL |
| ATOM | 674 | O | TYR | 82 | 19.217 | 42.804 | 117.421 | 1.00 | 12.93 | HIGL |
| ATOM | 675 | N | SER | 83 | 18.137 | 43.256 | 119.352 | 1.00 | 13.03 | HIGL |
| ATOM | 676 | CA | SER | 83 | 19.132 | 42.668 | 120.227 | 1.00 | 13.56 | HIGL |
| ATOM | 677 | CB | SER | 83 | 20.266 | 43.671 | 120.439 | 1.00 | 13.70 | HIGL |
| ATOM | 678 | OG | SER | 83 | 21.309 | 43.114 | 121.210 | 1.00 | 15.51 | HIGL |
| ATOM | 679 | C | SER | 83 | 18.440 | 42.348 | 121.557 | 1.00 | 14.03 | HIGL |
| ATOM | 680 | O | SER | 83 | 17.332 | 42.827 | 121.805 | 1.00 | 13.59 | HIGL |
| ATOM | 681 | N | ASP | 84 | 19.066 | 41.532 | 122.405 | 1.00 | 14.12 | HIGL |
| ATOM | 682 | CA | ASP | 84 | 18.453 | 41.215 | 123.694 | 1.00 | 14.35 | HIGL |
| ATOM | 683 | CB | ASP | 84 | 19.025 | 39.927 | 124.294 | 1.00 | 15.38 | HIGL |
| ATOM | 684 | CG | ASP | 84 | 18.577 | 38.682 | 123.558 | 1.00 | 16.47 | HIGL |
| ATOM | 685 | OD1 | ASP | 84 | 17.543 | 38.736 | 122.856 | 1.00 | 16.36 | HIGL |
| ATOM | 686 | OD2 | ASP | 84 | 19.259 | 37.643 | 123.704 | 1.00 | 17.16 | HIGL |
| ATOM | 687 | C | ASP | 84 | 18.760 | 42.357 | 124.640 | 1.00 | 13.54 | HIGL |
| ATOM | 688 | O | ASP | 84 | 18.066 | 42.571 | 125.629 | 1.00 | 12.95 | HIGL |
| ATOM | 689 | N | THR | 85 | 19.806 | 43.100 | 124.308 | 1.00 | 12.90 | HIGL |
| ATOM | 690 | CA | THR | 85 | 20.240 | 44.199 | 125.141 | 1.00 | 12.85 | HIGL |
| ATOM | 691 | CB | THR | 85 | 21.471 | 43.771 | 125.920 | 1.00 | 12.51 | HIGL |
| ATOM | 692 | OG1 | THR | 85 | 21.661 | 44.642 | 127.038 | 1.00 | 14.10 | HIGL |
| ATOM | 693 | CG2 | THR | 85 | 22.685 | 43.810 | 125.013 | 1.00 | 12.87 | HIGL |
| ATOM | 694 | C | THR | 85 | 20.555 | 45.453 | 124.314 | 1.00 | 12.72 | HIGL |
| ATOM | 695 | O | THR | 85 | 20.377 | 45.463 | 123.095 | 1.00 | 12.75 | HIGL |
| ATOM | 696 | N | TRP | 86 | 21.038 | 46.495 | 124.989 | 1.00 | 11.76 | HIGL |
| ATOM | 697 | CA | TRP | 86 | 21.358 | 47.772 | 124.354 | 1.00 | 10.89 | HIGL |
| ATOM | 698 | CB | TRP | 86 | 22.198 | 48.651 | 125.276 | 1.00 | 9.89 | HIGL |
| ATOM | 699 | CG | TRP | 86 | 21.597 | 48.938 | 126.604 | 1.00 | 10.03 | HIGL |
| ATOM | 700 | CD2 | TRP | 86 | 20.629 | 49.947 | 126.908 | 1.00 | 9.39 | HIGL |
| ATOM | 701 | CE2 | TRP | 86 | 20.363 | 49.865 | 128.292 | 1.00 | 8.31 | HIGL |
| ATOM | 702 | CE3 | TRP | 86 | 19.959 | 50.913 | 126.147 | 1.00 | 9.93 | HIGL |
| ATOM | 703 | CD1 | TRP | 86 | 21.870 | 48.302 | 127.781 | 1.00 | 8.33 | HIGL |
| ATOM | 704 | NE1 | TRP | 86 | 21.135 | 48.852 | 128.796 | 1.00 | 7.98 | HIGL |
| ATOM | 705 | CZ2 | TRP | 86 | 19.457 | 50.711 | 128.932 | 1.00 | 7.91 | HIGL |
| ATOM | 706 | CZ3 | TRP | 86 | 19.051 | 51.760 | 126.788 | 1.00 | 9.09 | HIGL |
| ATOM | 707 | CH2 | TRP | 86 | 18.812 | 51.649 | 128.166 | 1.00 | 9.37 | HIGL |
| ATOM | 708 | C | TRP | 86 | 22.111 | 47.668 | 123.048 | 1.00 | 11.73 | HIGL |
| ATOM | 709 | O | TRP | 86 | 23.216 | 47.141 | 123.008 | 1.00 | 11.69 | HIGL |
| ATOM | 710 | N | ALA | 87 | 21.524 | 48.193 | 121.980 | 1.00 | 12.59 | HIGL |
| ATOM | 711 | CA | ALA | 87 | 22.189 | 48.180 | 120.685 | 1.00 | 12.82 | HIGL |
| ATOM | 712 | CB | ALA | 87 | 21.246 | 47.706 | 119.603 | 1.00 | 12.18 | HIGL |
| ATOM | 713 | C | ALA | 87 | 22.665 | 49.594 | 120.381 | 1.00 | 13.67 | HIGL |
| ATOM | 714 | O | ALA | 87 | 21.912 | 50.553 | 120.532 | 1.00 | 13.58 | HIGL |

# Fig. 2 cont.

| ATOM | 715 | N   | ASP | 88 | 23.929 | 49.710 | 119.984 | 1.00 | 14.42 | HIGL |
|------|-----|-----|-----|----|--------|--------|---------|------|-------|------|
| ATOM | 716 | CA  | ASP | 88 | 24.538 | 50.984 | 119.628 | 1.00 | 14.58 | HIGL |
| ATOM | 717 | CB  | ASP | 88 | 24.990 | 51.744 | 120.889 | 1.00 | 14.68 | HIGL |
| ATOM | 718 | CG  | ASP | 88 | 25.901 | 50.925 | 121.783 | 1.00 | 16.21 | HIGL |
| ATOM | 719 | OD1 | ASP | 88 | 26.827 | 50.268 | 121.263 | 1.00 | 18.18 | HIGL |
| ATOM | 720 | OD2 | ASP | 88 | 25.701 | 50.949 | 123.014 | 1.00 | 16.03 | HIGL |
| ATOM | 721 | C   | ASP | 88 | 25.721 | 50.691 | 118.690 | 1.00 | 15.64 | HIGL |
| ATOM | 722 | O   | ASP | 88 | 26.023 | 49.529 | 118.416 | 1.00 | 15.14 | HIGL |
| ATOM | 723 | N   | PRO | 89 | 26.408 | 51.734 | 118.192 | 1.00 | 16.24 | HIGL |
| ATOM | 724 | CD  | PRO | 89 | 26.232 | 53.163 | 118.505 | 1.00 | 16.14 | HIGL |
| ATOM | 725 | CA  | PRO | 89 | 27.545 | 51.549 | 117.280 | 1.00 | 16.34 | HIGL |
| ATOM | 726 | CB  | PRO | 89 | 28.119 | 52.954 | 117.159 | 1.00 | 16.73 | HIGL |
| ATOM | 727 | CG  | PRO | 89 | 26.918 | 53.823 | 117.343 | 1.00 | 17.24 | HIGL |
| ATOM | 728 | C   | PRO | 89 | 28.607 | 50.541 | 117.708 | 1.00 | 16.16 | HIGL |
| ATOM | 729 | O   | PRO | 89 | 29.283 | 49.961 | 116.871 | 1.00 | 15.63 | HIGL |
| ATOM | 730 | N   | ALA | 90 | 28.760 | 50.326 | 119.006 | 1.00 | 16.46 | HIGL |
| ATOM | 731 | CA  | ALA | 90 | 29.773 | 49.387 | 119.462 | 1.00 | 16.48 | HIGL |
| ATOM | 732 | CB  | ALA | 90 | 30.596 | 50.003 | 120.598 | 1.00 | 14.72 | HIGL |
| ATOM | 733 | C   | ALA | 90 | 29.191 | 48.054 | 119.899 | 1.00 | 16.00 | HIGL |
| ATOM | 734 | O   | ALA | 90 | 29.939 | 47.143 | 120.241 | 1.00 | 17.19 | HIGL |
| ATOM | 735 | N   | HIS | 91 | 27.867 | 47.933 | 119.889 | 1.00 | 15.05 | HIGL |
| ATOM | 736 | CA  | HIS | 91 | 27.230 | 46.680 | 120.288 | 1.00 | 14.58 | HIGL |
| ATOM | 737 | CB  | HIS | 91 | 26.897 | 46.673 | 121.785 | 1.00 | 15.34 | HIGL |
| ATOM | 738 | CG  | HIS | 91 | 27.967 | 47.242 | 122.662 | 1.00 | 14.94 | HIGL |
| ATOM | 739 | CD2 | HIS | 91 | 28.755 | 46.663 | 123.599 | 1.00 | 15.42 | HIGL |
| ATOM | 740 | ND1 | HIS | 91 | 28.296 | 48.582 | 122.660 | 1.00 | 15.37 | HIGL |
| ATOM | 741 | CE1 | HIS | 91 | 29.237 | 48.803 | 123.561 | 1.00 | 16.41 | HIGL |
| ATOM | 742 | NE2 | HIS | 91 | 29.534 | 47.654 | 124.146 | 1.00 | 15.75 | HIGL |
| ATOM | 743 | C   | HIS | 91 | 25.939 | 46.414 | 119.518 | 1.00 | 14.68 | HIGL |
| ATOM | 744 | O   | HIS | 91 | 24.944 | 47.123 | 119.679 | 1.00 | 14.01 | HIGL |
| ATOM | 745 | N   | GLN | 92 | 25.968 | 45.385 | 118.680 | 1.00 | 14.89 | HIGL |
| ATOM | 746 | CA  | GLN | 92 | 24.818 | 44.974 | 117.885 | 1.00 | 14.67 | HIGL |
| ATOM | 747 | CB  | GLN | 92 | 25.000 | 45.394 | 116.421 | 1.00 | 13.95 | HIGL |
| ATOM | 748 | CG  | GLN | 92 | 24.928 | 46.904 | 116.159 | 1.00 | 13.75 | HIGL |
| ATOM | 749 | CD  | GLN | 92 | 23.529 | 47.497 | 116.368 | 1.00 | 13.63 | HIGL |
| ATOM | 750 | OE1 | GLN | 92 | 22.517 | 46.899 | 115.985 | 1.00 | 12.06 | HIGL |
| ATOM | 751 | NE2 | GLN | 92 | 23.475 | 48.685 | 116.958 | 1.00 | 11.96 | HIGL |
| ATOM | 752 | C   | GLN | 92 | 24.786 | 43.451 | 118.005 | 1.00 | 15.14 | HIGL |
| ATOM | 753 | O   | GLN | 92 | 24.994 | 42.721 | 117.033 | 1.00 | 14.92 | HIGL |
| ATOM | 754 | N   | THR | 93 | 24.530 | 42.984 | 119.222 | 1.00 | 15.07 | HIGL |
| ATOM | 755 | CA  | THR | 93 | 24.510 | 41.561 | 119.520 | 1.00 | 14.27 | HIGL |
| ATOM | 756 | CB  | THR | 93 | 24.672 | 41.329 | 121.023 | 1.00 | 14.39 | HIGL |
| ATOM | 757 | OG1 | THR | 93 | 25.783 | 42.100 | 121.497 | 1.00 | 13.20 | HIGL |
| ATOM | 758 | CG2 | THR | 93 | 24.906 | 39.842 | 121.315 | 1.00 | 12.37 | HIGL |
| ATOM | 759 | C   | THR | 93 | 23.259 | 40.838 | 119.070 | 1.00 | 15.03 | HIGL |
| ATOM | 760 | O   | THR | 93 | 22.169 | 41.066 | 119.600 | 1.00 | 15.53 | HIGL |
| ATOM | 761 | N   | THR | 94 | 23.428 | 39.951 | 118.097 | 1.00 | 14.94 | HIGL |
| ATOM | 762 | CA  | THR | 94 | 22.323 | 39.162 | 117.576 | 1.00 | 15.30 | HIGL |
| ATOM | 763 | CB  | THR | 94 | 22.818 | 38.169 | 116.503 | 1.00 | 15.55 | HIGL |
| ATOM | 764 | OG1 | THR | 94 | 23.376 | 38.893 | 115.399 | 1.00 | 15.22 | HIGL |
| ATOM | 765 | CG2 | THR | 94 | 21.677 | 37.302 | 116.013 | 1.00 | 15.52 | HIGL |
| ATOM | 766 | C   | THR | 94 | 21.720 | 38.373 | 118.732 | 1.00 | 15.67 | HIGL |
| ATOM | 767 | O   | THR | 94 | 22.447 | 37.830 | 119.563 | 1.00 | 15.25 | HIGL |
| ATOM | 768 | N   | PRO | 95 | 20.381 | 38.309 | 118.806 | 1.00 | 16.47 | HIGL |
| ATOM | 769 | CD  | PRO | 95 | 19.409 | 38.946 | 117.901 | 1.00 | 16.88 | HIGL |
| ATOM | 770 | CA  | PRO | 95 | 19.695 | 37.573 | 119.878 | 1.00 | 16.79 | HIGL |
| ATOM | 771 | CB  | PRO | 95 | 18.220 | 37.690 | 119.490 | 1.00 | 16.02 | HIGL |
| ATOM | 772 | CG  | PRO | 95 | 18.161 | 38.991 | 118.754 | 1.00 | 16.42 | HIGL |
| ATOM | 773 | C   | PRO | 95 | 20.156 | 36.119 | 119.896 | 1.00 | 17.32 | HIGL |
| ATOM | 774 | O   | PRO | 95 | 20.230 | 35.480 | 118.845 | 1.00 | 18.48 | HIGL |
| ATOM | 775 | N   | ALA | 96 | 20.472 | 35.590 | 121.073 | 1.00 | 17.31 | HIGL |
| ATOM | 776 | CA  | ALA | 96 | 20.903 | 34.196 | 121.149 | 1.00 | 17.43 | HIGL |
| ATOM | 777 | CB  | ALA | 96 | 21.086 | 33.769 | 122.598 | 1.00 | 17.13 | HIGL |
| ATOM | 778 | C   | ALA | 96 | 19.821 | 33.356 | 120.495 | 1.00 | 16.72 | HIGL |
| ATOM | 779 | O   | ALA | 96 | 18.636 | 33.612 | 120.693 | 1.00 | 15.96 | HIGL |

# Fig. 2 cont.

| ATOM | 780 | N | GLY | 97 | 20.229 | 32.371 | 119.700 | 1.00 | 17.32 | HIGL |
|------|-----|-----|-----|-----|--------|--------|---------|------|-------|------|
| ATOM | 781 | CA | GLY | 97 | 19.263 | 31.515 | 119.031 | 1.00 | 17.04 | HIGL |
| ATOM | 782 | C | GLY | 97 | 19.001 | 31.856 | 117.573 | 1.00 | 17.23 | HIGL |
| ATOM | 783 | O | GLY | 97 | 18.675 | 30.976 | 116.783 | 1.00 | 17.90 | HIGL |
| ATOM | 784 | N | TRP | 98 | 19.135 | 33.124 | 117.205 | 1.00 | 16.99 | HIGL |
| ATOM | 785 | CA | TRP | 98 | 18.907 | 33.524 | 115.820 | 1.00 | 17.97 | HIGL |
| ATOM | 786 | CB | TRP | 98 | 18.901 | 35.051 | 115.726 | 1.00 | 18.18 | HIGL |
| ATOM | 787 | CG | TRP | 98 | 17.627 | 35.621 | 116.258 | 1.00 | 18.37 | HIGL |
| ATOM | 788 | CD2 | TRP | 98 | 17.022 | 36.870 | 115.907 | 1.00 | 18.66 | HIGL |
| ATOM | 789 | CE2 | TRP | 98 | 15.824 | 36.978 | 116.650 | 1.00 | 18.98 | HIGL |
| ATOM | 790 | CE3 | TRP | 98 | 17.372 | 37.909 | 115.036 | 1.00 | 18.95 | HIGL |
| ATOM | 791 | CD1 | TRP | 98 | 16.798 | 35.041 | 117.175 | 1.00 | 18.96 | HIGL |
| ATOM | 792 | NE1 | TRP | 98 | 15.714 | 35.846 | 117.415 | 1.00 | 19.48 | HIGL |
| ATOM | 793 | CZ2 | TRP | 98 | 14.973 | 38.083 | 116.550 | 1.00 | 18.24 | HIGL |
| ATOM | 794 | CZ3 | TRP | 98 | 16.521 | 39.011 | 114.936 | 1.00 | 18.88 | HIGL |
| ATOM | 795 | CH2 | TRP | 98 | 15.336 | 39.085 | 115.690 | 1.00 | 18.43 | HIGL |
| ATOM | 796 | C | TRP | 98 | 19.939 | 32.897 | 114.877 | 1.00 | 17.57 | HIGL |
| ATOM | 797 | O | TRP | 98 | 21.042 | 32.569 | 115.285 | 1.00 | 17.56 | HIGL |
| ATOM | 798 | N | PRO | 99 | 19.577 | 32.707 | 113.601 | 1.00 | 17.79 | HIGL |
| ATOM | 799 | CD | PRO | 99 | 18.219 | 32.889 | 113.063 | 1.00 | 17.38 | HIGL |
| ATOM | 800 | CA | PRO | 99 | 20.459 | 32.106 | 112.594 | 1.00 | 17.62 | HIGL |
| ATOM | 801 | CB | PRO | 99 | 19.578 | 32.055 | 111.342 | 1.00 | 17.40 | HIGL |
| ATOM | 802 | CG | PRO | 99 | 18.491 | 33.041 | 111.616 | 1.00 | 18.07 | HIGL |
| ATOM | 803 | C | PRO | 99 | 21.842 | 32.693 | 112.326 | 1.00 | 17.38 | HIGL |
| ATOM | 804 | O | PRO | 99 | 22.147 | 33.820 | 112.709 | 1.00 | 17.86 | HIGL |
| ATOM | 805 | N | SER | 100 | 22.670 | 31.887 | 111.660 | 1.00 | 17.52 | HIGL |
| ATOM | 806 | CA | SER | 100 | 24.045 | 32.240 | 111.323 | 1.00 | 16.92 | HIGL |
| ATOM | 807 | CB | SER | 100 | 24.992 | 31.142 | 111.793 | 1.00 | 16.67 | HIGL |
| ATOM | 808 | OG | SER | 100 | 24.564 | 30.601 | 113.025 | 1.00 | 20.79 | HIGL |
| ATOM | 809 | C | SER | 100 | 24.283 | 32.452 | 109.833 | 1.00 | 16.73 | HIGL |
| ATOM | 810 | O | SER | 100 | 25.419 | 32.675 | 109.423 | 1.00 | 17.27 | HIGL |
| ATOM | 811 | N | ASP | 101 | 23.247 | 32.336 | 109.012 | 1.00 | 16.22 | HIGL |
| ATOM | 812 | CA | ASP | 101 | 23.422 | 32.564 | 107.579 | 1.00 | 16.38 | HIGL |
| ATOM | 813 | CB | ASP | 101 | 23.121 | 31.303 | 106.751 | 1.00 | 16.22 | HIGL |
| ATOM | 814 | CG | ASP | 101 | 21.708 | 30.805 | 106.929 | 1.00 | 15.46 | HIGL |
| ATOM | 815 | OD1 | ASP | 101 | 21.423 | 30.151 | 107.950 | 1.00 | 16.82 | HIGL |
| ATOM | 816 | OD2 | ASP | 101 | 20.877 | 31.073 | 106.047 | 1.00 | 16.15 | HIGL |
| ATOM | 817 | C | ASP | 101 | 22.494 | 33.707 | 107.201 | 1.00 | 16.52 | HIGL |
| ATOM | 818 | O | ASP | 101 | 21.387 | 33.825 | 107.736 | 1.00 | 16.54 | · HIGL |
| ATOM | 819 | N | ILE | 102 | 22.957 | 34.545 | 106.280 | 1.00 | 15.85 | HIGL |
| ATOM | 820 | CA | ILE | 102 | 22.220 | 35.727 | 105.871 | 1.00 | 15.30 | HIGL |
| ATOM | 821 | CB | ILE | 102 | 22.958 | 36.484 | 104.746 | 1.00 | 14.62 | HIGL |
| ATOM | 822 | CG2 | ILE | 102 | 22.862 | 35.709 | 103.433 | 1.00 | 14.59 | HIGL |
| ATOM | 823 | CG1 | ILE | 102 | 22.361 | 37.884 | 104.594 | 1.00 | 13.26 | HIGL |
| ATOM | 824 | CD1 | ILE | 102 | 22.438 | 38.731 | 105.856 | 1.00 | 10.57 | HIGL |
| ATOM | 825 | C | ILE | 102 | 20.779 | 35.519 | 105.452 | 1.00 | 16.31 | HIGL |
| ATOM | 826 | O | ILE | 102 | 19.929 | 36.365 | 105.739 | 1.00 | 17.53 | HIGL |
| ATOM | 827 | N | ASN | 103 | 20.486 | 34.409 | 104.784 | 1.00 | 15.84 | HIGL |
| ATOM | 828 | CA | ASN | 103 | 19.118 | 34.174 | 104.347 | 1.00 | 15.26 | HIGL |
| ATOM | 829 | CB | ASN | 103 | 19.056 | 33.026 | 103.345 | 1.00 | 16.44 | HIGL |
| ATOM | 830 | CG | ASN | 103 | 17.643 | 32.754 | 102.881 | 1.00 | 17.90 | HIGL |
| ATOM | 831 | OD1 | ASN | 103 | 17.012 | 33.606 | 102.251 | 1.00 | 17.31 | HIGL |
| ATOM | 832 | ND2 | ASN | 103 | 17.128 | 31.568 | 103.207 | 1.00 | 18.73 | HIGL |
| ATOM | 833 | C | ASN | 103 | 18.195 | 33.872 | 105.520 | 1.00 | 14.76 | HIGL |
| ATOM | 834 | O | ASN | 103 | 17.081 | 34.390 | 105.592 | 1.00 | 14.43 | HIGL |
| ATOM | 835 | N | ASN | 104 | 18.655 | 33.029 | 106.437 | 1.00 | 14.10 | HIGL |
| ATOM | 836 | CA | ASN | 104 | 17.849 | 32.684 | 107.598 | 1.00 | 13.79 | HIGL |
| ATOM | 837 | CB | ASN | 104 | 18.391 | 31.424 | 108.277 | 1.00 | 13.76 | HIGL |
| ATOM | 838 | CG | ASN | 104 | 17.923 | 30.149 | 107.594 | 1.00 | 14.35 | HIGL |
| ATOM | 839 | OD1 | ASN | 104 | 16.738 | 30.006 | 107.264 | 1.00 | 13.83 | HIGL |
| ATOM | 840 | ND2 | ASN | 104 | 18.843 | 29.212 | 107.392 | 1.00 | 11.49 | HIGL |
| ATOM | 841 | C | ASN | 104 | 17.766 | 33.822 | 108.603 | 1.00 | 13.46 | HIGL |
| ATOM | 842 | O | ASN | 104 | 16.706 | 34.066 | 109.169 | 1.00 | 13.67 | HIGL |
| ATOM | 843 | N | LEU | 105 | 18.875 | 34.522 | 108.824 | 1.00 | 13.84 | HIGL |
| ATOM | 844 | CA | LEU | 105 | 18.885 | 35.640 | 109.762 | 1.00 | 14.45 | HIGL |

# Fig. 2 cont.

| ATOM | 845 | CB | LEU | 105 | 20.282 | 36.256 | 109.855 | 1.00 | 14.35 | HIGL |
|------|-----|-----|-----|-----|--------|--------|---------|------|-------|------|
| ATOM | 846 | CG | LEU | 105 | 20.373 | 37.492 | 110.754 | 1.00 | 15.28 | HIGL |
| ATOM | 847 | CD1 | LEU | 105 | 19.941 | 37.133 | 112.168 | 1.00 | 14.98 | HIGL |
| ATOM | 848 | CD2 | LEU | 105 | 21.791 | 38.025 | 110.756 | 1.00 | 15.43 | HIGL |
| ATOM | 849 | C | LEU | 105 | 17.891 | 36.694 | 109.291 | 1.00 | 15.25 | HIGL |
| ATOM | 850 | O | LEU | 105 | 17.087 | 37.204 | 110.074 | 1.00 | 14.19 | HIGL |
| ATOM | 851 | N | ALA | 106 | 17.956 | 37.009 | 108.000 | 1.00 | 15.85 | HIGL |
| ATOM | 852 | CA | ALA | 106 | 17.067 | 37.990 | 107.399 | 1.00 | 17.40 | HIGL |
| ATOM | 853 | CB | ALA | 106 | 17.417 | 38.177 | 105.916 | 1.00 | 15.61 | HIGL |
| ATOM | 854 | C | ALA | 106 | 15.618 | 37.532 | 107.548 | 1.00 | 18.34 | HIGL |
| ATOM | 855 | O | ALA | 106 | 14.730 | 38.326 | 107.859 | 1.00 | 19.25 | HIGL |
| ATOM | 856 | N | TRP | 107 | 15.390 | 36.245 | 107.320 | 1.00 | 19.52 | HIGL |
| ATOM | 857 | CA | TRP | 107 | 14.060 | 35.663 | 107.430 | 1.00 | 20.70 | HIGL |
| ATOM | 858 | CB | TRP | 107 | 14.140 | 34.177 | 107.104 | 1.00 | 22.69 | HIGL |
| ATOM | 859 | CG | TRP | 107 | 12.847 | 33.566 | 106.709 | 1.00 | 26.10 | HIGL |
| ATOM | 860 | CD2 | TRP | 107 | 12.607 | 32.179 | 106.453 | 1.00 | 27.36 | HIGL |
| ATOM | 861 | CE2 | TRP | 107 | 11.256 | 32.056 | 106.055 | 1.00 | 28.11 | HIGL |
| ATOM | 862 | CE3 | TRP | 107 | 13.404 | 31.028 | 106.517 | 1.00 | 27.84 | HIGL |
| ATOM | 863 | CD1 | TRP | 107 | 11.665 | 34.212 | 106.466 | 1.00 | 26.98 | HIGL |
| ATOM | 864 | NE1 | TRP | 107 | 10.705 | 33.310 | 106.072 | 1.00 | 27.36 | HIGL |
| ATOM | 865 | CZ2 | TRP | 107 | 10.683 | 30.821 | 105.720 | 1.00 | 28.94 | HIGL |
| ATOM | 866 | CZ3 | TRP | 107 | 12.836 | 29.804 | 106.184 | 1.00 | 28.94 | HIGL |
| ATOM | 867 | CH2 | TRP | 107 | 11.487 | 29.711 | 105.790 | 1.00 | 28.79 | HIGL |
| ATOM | 868 | C | TRP | 107 | 13.567 | 35.862 | 108.862 | 1.00 | 20.80 | HIGL |
| ATOM | 869 | O | TRP | 107 | 12.428 | 36.280 | 109.097 | 1.00 | 19.49 | HIGL |
| ATOM | 870 | N | LYS | 108 | 14.453 | 35.567 | 109.812 | 1.00 | 20.81 | HIGL |
| ATOM | 871 | CA | LYS | 108 | 14.158 | 35.707 | 111.231 | 1.00 | 20.77 | HIGL |
| ATOM | 872 | CB | LYS | 108 | 15.358 | 35.255 | 112.070 | 1.00 | 21.15 | HIGL |
| ATOM | 873 | CG | LYS | 108 | 15.018 | 34.250 | 113.161 | 1.00 | 22.88 | HIGL |
| ATOM | 874 | CD | LYS | 108 | 13.942 | 34.770 | 114.100 | 1.00 | 23.37 | HIGL |
| ATOM | 875 | CE | LYS | 108 | 13.525 | 33.698 | 115.088 | 1.00 | 23.83 | HIGL |
| ATOM | 876 | NZ | LYS | 108 | 12.322 | 34.107 | 115.853 | 1.00 | 24.90 | HIGL |
| ATOM | 877 | C | LYS | 108 | 13.830 | 37.161 | 111.554 | 1.00 | 19.90 | HIGL |
| ATOM | 878 | O | LYS | 108 | 12.836 | 37.450 | 112.214 | 1.00 | 20.08 | HIGL |
| ATOM | 879 | N | LEU | 109 | 14.674 | 38.074 | 111.094 | 1.00 | 19.75 | HIGL |
| ATOM | 880 | CA | LEU | 109 | 14.445 | 39.488 | 111.344 | 1.00 | 19.93 | HIGL |
| ATOM | 881 | CB | LEU | 109 | 15.508 | 40.337 | 110.654 | 1.00 | 17.82 | HIGL |
| ATOM | 882 | CG | LEU | 109 | 15.390 | 41.827 | 110.968 | 1.00 | 17.82 | HIGL |
| ATOM | 883 | CD1 | LEU | 109 | 15.672 | 42.054 | 112.449 | 1.00 | 16.38 | HIGL |
| ATOM | 884 | CD2 | LEU | 109 | 16.368 | 42.620 | 110.103 | 1.00 | 16.81 | HIGL |
| ATOM | 885 | C | LEU | 109 | 13.063 | 39.861 | 110.822 | 1.00 | 20.34 | HIGL |
| ATOM | 886 | O | LEU | 109 | 12.362 | 40.679 | 111.423 | 1.00 | 20.28 | HIGL |
| ATOM | 887 | N | TYR | 110 | 12.679 | 39.247 | 109.704 | 1.00 | 20.51 | HIGL |
| ATOM | 888 | CA | TYR | 110 | 11.377 | 39.489 | 109.100 | 1.00 | 20.92 | HIGL |
| ATOM | 889 | CB | TYR | 110 | 11.309 | 38.862 | 107.704 | 1.00 | 21.24 | HIGL |
| ATOM | 890 | CG | TYR | 110 | 9.918 | 38.842 | 107.101 | 1.00 | 21.40 | HIGL |
| ATOM | 891 | CD1 | TYR | 110 | 9.064 | 37.757 | 107.292 | 1.00 | 22.61 | HIGL |
| ATOM | 892 | CE1 | TYR | 110 | 7.771 | 37.748 | 106.754 | 1.00 | 22.76 | HIGL |
| ATOM | 893 | CD2 | TYR | 110 | 9.445 | 39.922 | 106.358 | 1.00 | 23.16 | HIGL |
| ATOM | 894 | CE2 | TYR | 110 | 8.155 | 39.926 | 105.817 | 1.00 | 22.90 | HIGL |
| ATOM | 895 | CZ | TYR | 110 | 7.325 | 38.838 | 106.018 | 1.00 | 23.09 | HIGL |
| ATOM | 896 | OH | TYR | 110 | 6.056 | 38.849 | 105.482 | 1.00 | 22.70 | HIGL |
| ATOM | 897 | C | TYR | 110 | 10.249 | 38.938 | 109.972 | 1.00 | 21.45 | HIGL |
| ATOM | 898 | O | TYR | 110 | 9.312 | 39.671 | 110.303 | 1.00 | 22.10 | HIGL |
| ATOM | 899 | N | ASN | 111 | 10.326 | 37.659 | 110.344 | 1.00 | 20.73 | HIGL |
| ATOM | 900 | CA | ASN | 111 | 9.281 | 37.073 | 111.182 | 1.00 | 20.87 | HIGL |
| ATOM | 901 | CB | ASN | 111 | 9.589 | 35.619 | 111.546 | 1.00 | 23.22 | HIGL |
| ATOM | 902 | CG | ASN | 111 | 9.612 | 34.699 | 110.348 | 1.00 | 26.49 | HIGL |
| ATOM | 903 | OD1 | ASN | 111 | 9.040 | 35.005 | 109.301 | 1.00 | 27.21 | HIGL |
| ATOM | 904 | ND2 | ASN | 111 | 10.265 | 33.552 | 110.516 | 1.00 | 29.16 | HIGL |
| ATOM | 905 | C | ASN | 111 | 9.147 | 37.864 | 112.474 | 1.00 | 19.60 | HIGL |
| ATOM | 906 | O | ASN | 111 | 8.039 | 38.190 | 112.905 | 1.00 | 19.02 | HIGL |
| ATOM | 907 | N | TYR | 112 | 10.288 | 38.169 | 113.084 | 1.00 | 18.21 | HIGL |
| ATOM | 908 | CA | TYR | 112 | 10.310 | 38.905 | 114.337 | 1.00 | 16.83 | HIGL |
| ATOM | 909 | CB | TYR | 112 | 11.751 | 39.129 | 114.810 | 1.00 | 16.36 | HIGL |

# Fig. 2 cont.

| ATOM | 910 | CG | TYR | 112 | 11.839 | 40.071 | 115.991 | 1.00 | 14.95 | HIGL |
|------|-----|-----|-----|-----|--------|--------|---------|------|-------|------|
| ATOM | 911 | CD1 | TYR | 112 | 11.369 | 39.691 | 117.245 | 1.00 | 15.11 | HIGL |
| ATOM | 912 | CE1 | TYR | 112 | 11.369 | 40.581 | 118.316 | 1.00 | 14.94 | HIGL |
| ATOM | 913 | CD2 | TYR | 112 | 12.319 | 41.366 | 115.836 | 1.00 | 14.45 | HIGL |
| ATOM | 914 | CE2 | TYR | 112 | 12.323 | 42.264 | 116.897 | 1.00 | 14.83 | HIGL |
| ATOM | 915 | CZ | TYR | 112 | 11.847 | 41.866 | 118.133 | 1.00 | 14.96 | HIGL |
| ATOM | 916 | OH | TYR | 112 | 11.848 | 42.754 | 119.182 | 1.00 | 15.27 | HIGL |
| ATOM | 917 | C | TYR | 112 | 9.601 | 40.243 | 114.224 | 1.00 | 16.36 | HIGL |
| ATOM | 918 | O | TYR | 112 | 8.686 | 40.534 | 114.999 | 1.00 | 15.41 | HIGL |
| ATOM | 919 | N | THR | 113 | 10.034 | 41.056 | 113.265 | 1.00 | 16.21 | HIGL |
| ATOM | 920 | CA | THR | 113 | 9.443 | 42.369 | 113.058 | 1.00 | 15.87 | HIGL |
| ATOM | 921 | CB | THR | 113 | 10.142 | 43.125 | 111.922 | 1.00 | 16.16 | HIGL |
| ATOM | 922 | OG1 | THR | 113 | 11.537 | 43.252 | 112.221 | 1.00 | 15.12 | HIGL |
| ATOM | 923 | CG2 | THR | 113 | 9.537 | 44.515 | 111.758 | 1.00 | 15.98 | HIGL |
| ATOM | 924 | C | THR | 113 | 7.973 | 42.216 | 112.717 | 1.00 | 16.24 | HIGL |
| ATOM | 925 | O | THR | 113 | 7.124 | 42.896 | 113.290 | 1.00 | 16.57 | HIGL |
| ATOM | 926 | N | LEU | 114 | 7.678 | 41.307 | 111.790 | 1.00 | 16.92 | HIGL |
| ATOM | 927 | CA | LEU | 114 | 6.304 | 41.043 | 111.366 | 1.00 | 16.65 | HIGL |
| ATOM | 928 | CB | LEU | 114 | 6.264 | 39.849 | 110.411 | 1.00 | 15.97 | HIGL |
| ATOM | 929 | CG | LEU | 114 | 4.861 | 39.423 | 109.964 | 1.00 | 16.54 | HIGL |
| ATOM | 930 | CD1 | LEU | 114 | 4.220 | 40.543 | 109.154 | 1.00 | 15.93 | HIGL |
| ATOM | 931 | CD2 | LEU | 114 | 4.948 | 38.144 | 109.146 | 1.00 | 14.91 | HIGL |
| ATOM | 932 | C | LEU | 114 | 5.404 | 40.754 | 112.565 | 1.00 | 16.56 | HIGL |
| ATOM | 933 | O | LEU | 114 | 4.420 | 41.450 | 112.799 | 1.00 | 16.01 | HIGL |
| ATOM | 934 | N | ASP | 115 | 5.749 | 39.720 | 113.320 | 1.00 | 16.95 | HIGL |
| ATOM | 935 | CA | ASP | 115 | 4.967 | 39.347 | 114.484 | 1.00 | 17.44 | HIGL |
| ATOM | 936 | CB | ASP | 115 | 5.562 | 38.104 | 115.139 | 1.00 | 18.68 | HIGL |
| ATOM | 937 | CG | ASP | 115 | 5.489 | 36.884 | 114.235 | 1.00 | 20.91 | HIGL |
| ATOM | 938 | OD1 | ASP | 115 | 4.994 | 37.019 | 113.095 | 1.00 | 20.18 | HIGL |
| ATOM | 939 | OD2 | ASP | 115 | 5.928 | 35.789 | 114.658 | 1.00 | 22.87 | HIGL |
| ATOM | 940 | C | ASP | 115 | 4.879 | 40.481 | 115.491 | 1.00 | 17.05 | HIGL |
| ATOM | 941 | O | ASP | 115 | 3.813 | 40.732 | 116.048 | 1.00 | 16.42 | HIGL |
| ATOM | 942 | N | SER | 116 | 5.990 | 41.174 | 115.713 | 1.00 | 16.71 | HIGL |
| ATOM | 943 | CA | SER | 116 | 6.005 | 42.279 | 116.660 | 1.00 | 17.19 | HIGL |
| ATOM | 944 | CB | SER | 116 | 7.409 | 42.869 | 116.774 | 1.00 | 17.37 | HIGL |
| ATOM | 945 | OG | SER | 116 | 8.307 | 41.969 | 117.391 | 1.00 | 17.53 | HIGL |
| ATOM | 946 | C | SER | 116 | 5.023 | 43.381 | 116.262 | 1.00 | 18.12 | HIGL |
| ATOM | 947 | O | SER | 116 | 4.231 | 43.847 | 117.084 | 1.00 | 17.59 | HIGL |
| ATOM | 948 | N | MET | 117 | 5.080 | 43.812 | 115.008 | 1.00 | 18.86 | HIGL |
| ATOM | 949 | CA | MET | 117 | 4.176 | 44.856 | 114.552 | 1.00 | 19.77 | HIGL |
| ATOM | 950 | CB | MET | 117 | 4.525 | 45.262 | 113.125 | 1.00 | 19.25 | HIGL |
| ATOM | 951 | CG | MET | 117 | 5.862 | 45.989 | 113.006 | 1.00 | 18.96 | HIGL |
| ATOM | 952 | SD | MET | 117 | 5.846 | 47.687 | 113.654 | 1.00 | 20.56 | HIGL |
| ATOM | 953 | CE | MET | 117 | 6.173 | 47.395 | 115.398 | 1.00 | 20.80 | HIGL |
| ATOM | 954 | C | MET | 117 | 2.729 | 44.384 | 114.641 | 1.00 | 20.69 | HIGL |
| ATOM | 955 | O | MET | 117 | 1.843 | 45.134 | 115.056 | 1.00 | 19.86 | HIGL |
| ATOM | 956 | N | ASN | 118 | 2.488 | 43.132 | 114.266 | 1.00 | 22.17 | HIGL |
| ATOM | 957 | CA | ASN | 118 | 1.137 | 42.589 | 114.327 | 1.00 | 23.55 | HIGL |
| ATOM | 958 | CB | ASN | 118 | 1.081 | 41.192 | 113.704 | 1.00 | 22.99 | HIGL |
| ATOM | 959 | CG | ASN | 118 | 0.966 | 41.236 | 112.197 | 1.00 | 24.24 | HIGL |
| ATOM | 960 | OD1 | ASN | 118 | 0.231 | 42.054 | 111.648 | 1.00 | 24.38 | HIGL |
| ATOM | 961 | ND2 | ASN | 118 | 1.680 | 40.345 | 111.516 | 1.00 | 25.71 | HIGL |
| ATOM | 962 | C | ASN | 118 | 0.665 | 42.536 | 115.772 | 1.00 | 24.12 | HIGL |
| ATOM | 963 | O | ASN | 118 | -0.532 | 42.535 | 116.054 | 1.00 | 24.65 | HIGL |
| ATOM | 964 | N | ARG | 119 | 1.617 | 42.501 | 116.691 | 1.00 | 25.04 | HIGL |
| ATOM | 965 | CA | ARG | 119 | 1.289 | 42.457 | 118.104 | 1.00 | 25.97 | HIGL |
| ATOM | 966 | CB | ARG | 119 | 2.564 | 42.289 | 118.916 | 1.00 | 27.25 | HIGL |
| ATOM | 967 | CG | ARG | 119 | 2.324 | 41.905 | 120.343 | 1.00 | 30.86 | HIGL |
| ATOM | 968 | CD | ARG | 119 | 1.727 | 40.518 | 120.464 | 1.00 | 32.19 | HIGL |
| ATOM | 969 | NE | ARG | 119 | 1.381 | 40.252 | 121.856 | 1.00 | 35.20 | HIGL |
| ATOM | 970 | CZ | ARG | 119 | 2.266 | 40.036 | 122.826 | 1.00 | 35.79 | HIGL |
| ATOM | 971 | NH1 | ARG | 119 | 3.566 | 40.038 | 122.564 | 1.00 | 35.68 | HIGL |
| ATOM | 972 | NH2 | ARG | 119 | 1.845 | 39.846 | 124.070 | 1.00 | 37.32 | HIGL |
| ATOM | 973 | C | ARG | 119 | 0.572 | 43.755 | 118.483 | 1.00 | 26.06 | HIGL |
| ATOM | 974 | O | ARG | 119 | -0.406 | 43.744 | 119.234 | 1.00 | 26.17 | HIGL |

# Fig. 2 cont.

| ATOM | 975 | N | PHE | 120 | 1.058 | 44.874 | 117.952 | 1.00 | 25.97 | HIGL |
|------|------|------|-----|-----|--------|--------|---------|------|-------|------|
| ATOM | 976 | CA | PHE | 120 | 0.438 | 46.166 | 118.218 | 1.00 | 25.91 | HIGL |
| ATOM | 977 | CB | PHE | 120 | 1.369 | 47.312 | 117.811 | 1.00 | 24.71 | HIGL |
| ATOM | 978 | CG | PHE | 120 | 2.516 | 47.519 | 118.748 | 1.00 | 23.82 | HIGL |
| ATOM | 979 | CD1 | PHE | 120 | 3.748 | 46.923 | 118.508 | 1.00 | 24.05 | HIGL |
| ATOM | 980 | CD2 | PHE | 120 | 2.356 | 48.289 | 119.892 | 1.00 | 23.49 | HIGL |
| ATOM | 981 | CE1 | PHE | 120 | 4.806 | 47.088 | 119.396 | 1.00 | 23.14 | HIGL |
| ATOM | 982 | CE2 | PHE | 120 | 3.407 | 48.461 | 120.788 | 1.00 | 23.31 | HIGL |
| ATOM | 983 | CZ | PHE | 120 | 4.632 | 47.860 | 120.540 | 1.00 | 23.49 | HIGL |
| ATOM | 984 | C | PHE | 120 | −0.879 | 46.283 | 117.452 | 1.00 | 26.35 | HIGL |
| ATOM | 985 | O | PHE | 120 | −1.879 | 46.758 | 117.988 | 1.00 | 26.78 | HIGL |
| ATOM | 986 | N | ALA | 121 | −0.870 | 45.844 | 116.198 | 1.00 | 26.40 | HIGL |
| ATOM | 987 | CA | ALA | 121 | −2.058 | 45.891 | 115.357 | 1.00 | 26.80 | HIGL |
| ATOM | 988 | CB | ALA | 121 | −1.755 | 45.280 | 114.003 | 1.00 | 27.18 | HIGL |
| ATOM | 989 | C | ALA | 121 | −3.211 | 45.143 | 116.016 | 1.00 | 27.34 | HIGL |
| ATOM | 990 | O | ALA | 121 | −4.314 | 45.674 | 116.152 | 1.00 | 27.77 | HIGL |
| ATOM | 991 | N | ASP | 122 | −2.948 | 43.905 | 116.423 | 1.00 | 26.89 | HIGL |
| ATOM | 992 | CA | ASP | 122 | −3.965 | 43.084 | 117.063 | 1.00 | 26.21 | HIGL |
| ATOM | 993 | CB | ASP | 122 | −3.436 | 41.665 | 117.303 | 1.00 | 25.67 | HIGL |
| ATOM | 994 | CG | ASP | 122 | −3.074 | 40.950 | 116.012 | 1.00 | 25.38 | HIGL |
| ATOM | 995 | OD1 | ASP | 122 | −3.544 | 41.379 | 114.929 | 1.00 | 24.57 | HIGL |
| ATOM | 996 | OD2 | ASP | 122 | −2.328 | 39.950 | 116.089 | 1.00 | 24.15 | HIGL |
| ATOM | 997 | C | ASP | 122 | −4.414 | 43.686 | 118.389 | 1.00 | 26.13 | HIGL |
| ATOM | 998 | O | ASP | 122 | −5.549 | 43.478 | 118.822 | 1.00 | 26.95 | HIGL |
| ATOM | 999 | N | ALA | 123 | −3.517 | 44.427 | 119.033 | 1.00 | 24.90 | HIGL |
| ATOM | 1000 | CA | ALA | 123 | −3.821 | 45.053 | 120.308 | 1.00 | 22.75 | HIGL |
| ATOM | 1001 | CB | ALA | 123 | −2.548 | 45.330 | 121.058 | 1.00 | 23.23 | HIGL |
| ATOM | 1002 | C | ALA | 123 | −4.595 | 46.344 | 120.102 | 1.00 | 22.12 | HIGL |
| ATOM | 1003 | O | ALA | 123 | −5.085 | 46.935 | 121.058 | 1.00 | 22.33 | HIGL |
| ATOM | 1004 | N | GLY | 124 | −4.704 | 46.778 | 118.850 | 1.00 | 21.85 | HIGL |
| ATOM | 1005 | CA | GLY | 124 | −5.424 | 48.002 | 118.548 | 1.00 | 21.93 | HIGL |
| ATOM | 1006 | C | GLY | 124 | −4.604 | 49.253 | 118.809 | 1.00 | 22.90 | HIGL |
| ATOM | 1007 | O | GLY | 124 | −5.150 | 50.350 | 118.957 | 1.00 | 22.21 | HIGL |
| ATOM | 1008 | N | ILE | 125 | −3.286 | 49.078 | 118.876 | 1.00 | 23.51 | HIGL |
| ATOM | 1009 | CA | ILE | 125 | −2.352 | 50.174 | 119.113 | 1.00 | 23.71 | HIGL |
| ATOM | 1010 | CB | ILE | 125 | −1.132 | 49.706 | 119.949 | 1.00 | 24.28 | HIGL |
| ATOM | 1011 | CG2 | ILE | 125 | −0.171 | 50.871 | 120.153 | 1.00 | 22.68 | HIGL |
| ATOM | 1012 | CG1 | ILE | 125 | −1.587 | 49.094 | 121.283 | 1.00 | 24.08 | HIGL |
| ATOM | 1013 | CD1 | ILE | 125 | −2.168 | 50.078 | 122.258 | 1.00 | 24.75 | HIGL |
| ATOM | 1014 | C | ILE | 125 | −1.817 | 50.648 | 117.765 | 1.00 | 24.07 | HIGL |
| ATOM | 1015 | O | ILE | 125 | −1.416 | 49.837 | 116.939 | 1.00 | 24.23 | HIGL |
| ATOM | 1016 | N | GLN | 126 | −1.805 | 51.952 | 117.533 | 1.00 | 24.42 | HIGL |
| ATOM | 1017 | CA | GLN | 126 | −1.282 | 52.451 | 116.274 | 1.00 | 25.40 | HIGL |
| ATOM | 1018 | CB | GLN | 126 | −2.112 | 53.631 | 115.766 | 1.00 | 26.92 | HIGL |
| ATOM | 1019 | CG | GLN | 126 | −1.591 | 54.243 | 114.464 | 1.00 | 29.76 | HIGL |
| ATOM | 1020 | CD | GLN | 126 | −1.473 | 53.223 | 113.329 | 1.00 | 32.33 | HIGL |
| ATOM | 1021 | OE1 | GLN | 126 | −2.456 | 52.570 | 112.953 | 1.00 | 33.86 | HIGL |
| ATOM | 1022 | NE2 | GLN | 126 | −0.267 | 53.086 | 112.777 | 1.00 | 31.82 | HIGL |
| ATOM | 1023 | C | GLN | 126 | 0.174 | 52.883 | 116.424 | 1.00 | 25.09 | HIGL |
| ATOM | 1024 | O | GLN | 126 | 0.494 | 53.731 | 117.260 | 1.00 | 25.29 | HIGL |
| ATOM | 1025 | N | VAL | 127 | 1.046 | 52.280 | 115.617 | 1.00 | 23.64 | HIGL |
| ATOM | 1026 | CA | VAL | 127 | 2.465 | 52.605 | 115.614 | 1.00 | 21.87 | HIGL |
| ATOM | 1027 | CB | VAL | 127 | 3.329 | 51.373 | 115.255 | 1.00 | 21.30 | HIGL |
| ATOM | 1028 | CG1 | VAL | 127 | 4.800 | 51.730 | 115.338 | 1.00 | 20.09 | HIGL |
| ATOM | 1029 | CG2 | VAL | 127 | 3.010 | 50.217 | 116.184 | 1.00 | 20.69 | HIGL |
| ATOM | 1030 | C | VAL | 127 | 2.635 | 53.658 | 114.526 | 1.00 | 21.93 | HIGL |
| ATOM | 1031 | O | VAL | 127 | 2.268 | 53.427 | 113.378 | 1.00 | 22.89 | HIGL |
| ATOM | 1032 | N | ASP | 128 | 3.192 | 54.809 | 114.882 | 1.00 | 21.66 | HIGL |
| ATOM | 1033 | CA | ASP | 128 | 3.378 | 55.896 | 113.927 | 1.00 | 21.09 | HIGL |
| ATOM | 1034 | CB | ASP | 128 | 3.080 | 57.211 | 114.628 | 1.00 | 21.65 | HIGL |
| ATOM | 1035 | CG | ASP | 128 | 1.662 | 57.260 | 115.145 | 1.00 | 22.08 | HIGL |
| ATOM | 1036 | OD1 | ASP | 128 | 0.744 | 57.299 | 114.301 | 1.00 | 23.35 | HIGL |
| ATOM | 1037 | OD2 | ASP | 128 | 1.458 | 57.231 | 116.380 | 1.00 | 22.69 | HIGL |
| ATOM | 1038 | C | ASP | 128 | 4.746 | 55.932 | 113.256 | 1.00 | 21.00 | HIGL |
| ATOM | 1039 | O | ASP | 128 | 4.854 | 56.276 | 112.077 | 1.00 | 20.64 | HIGL |

# Fig. 2 cont.

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1040 | N | ILE | 129 | 5.786 | 55.587 | 114.010 | 1.00 | 19.93 | HIGL |
| ATOM | 1041 | CA | ILE | 129 | 7.139 | 55.535 | 113.472 | 1.00 | 18.94 | HIGL |
| ATOM | 1042 | CB | ILE | 129 | 7.999 | 56.721 | 113.927 | 1.00 | 17.89 | HIGL |
| ATOM | 1043 | CG2 | ILE | 129 | 9.425 | 56.533 | 113.444 | 1.00 | 16.07 | HIGL |
| ATOM | 1044 | CG1 | ILE | 129 | 7.440 | 58.027 | 113.375 | 1.00 | 17.25 | HIGL |
| ATOM | 1045 | CD1 | ILE | 129 | 8.207 | 59.241 | 113.843 | 1.00 | 16.76 | HIGL |
| ATOM | 1046 | C | ILE | 129 | 7.808 | 54.267 | 113.985 | 1.00 | 19.57 | HIGL |
| ATOM | 1047 | O | ILE | 129 | 7.591 | 53.867 | 115.130 | 1.00 | 20.12 | HIGL |
| ATOM | 1048 | N | VAL | 130 | 8.614 | 53.640 | 113.133 | 1.00 | 19.09 | HIGL |
| ATOM | 1049 | CA | VAL | 130 | 9.343 | 52.430 | 113.497 | 1.00 | 18.61 | HIGL |
| ATOM | 1050 | CB | VAL | 130 | 8.734 | 51.154 | 112.868 | 1.00 | 19.46 | HIGL |
| ATOM | 1051 | CG1 | VAL | 130 | 9.424 | 49.923 | 113.431 | 1.00 | 18.88 | HIGL |
| ATOM | 1052 | CG2 | VAL | 130 | 7.255 | 51.087 | 113.133 | 1.00 | 21.50 | HIGL |
| ATOM | 1053 | C | VAL | 130 | 10.762 | 52.531 | 112.962 | 1.00 | 17.57 | HIGL |
| ATOM | 1054 | O | VAL | 130 | 10.962 | 52.707 | 111.759 | 1.00 | 17.98 | HIGL |
| ATOM | 1055 | N | SER | 131 | 11.749 | 52.439 | 113.843 | 1.00 | 15.84 | HIGL |
| ATOM | 1056 | CA | SER | 131 | 13.127 | 52.470 | 113.377 | 1.00 | 14.70 | HIGL |
| ATOM | 1057 | CB | SER | 131 | 14.038 | 53.282 | 114.314 | 1.00 | 15.28 | HIGL |
| ATOM | 1058 | OG | SER | 131 | 14.319 | 52.589 | 115.514 | 1.00 | 18.11 | HIGL |
| ATOM | 1059 | C | SER | 131 | 13.565 | 51.018 | 113.345 | 1.00 | 12.96 | HIGL |
| ATOM | 1060 | O | SER | 131 | 13.436 | 50.299 | 114.335 | 1.00 | 11.68 | HIGL |
| ATOM | 1061 | N | ILE | 132 | 14.039 | 50.572 | 112.191 | 1.00 | 10.75 | HIGL |
| ATOM | 1062 | CA | ILE | 132 | 14.492 | 49.207 | 112.073 | 1.00 | 10.19 | HIGL |
| ATOM | 1063 | CB | ILE | 132 | 14.319 | 48.707 | 110.632 | 1.00 | 10.00 | HIGL |
| ATOM | 1064 | CG2 | ILE | 132 | 12.858 | 48.371 | 110.380 | 1.00 | 9.71 | HIGL |
| ATOM | 1065 | CG1 | ILE | 132 | 14.785 | 49.781 | 109.646 | 1.00 | 10.09 | HIGL |
| ATOM | 1066 | CD1 | ILE | 132 | 14.716 | 49.350 | 108.198 | 1.00 | 10.00 | HIGL |
| ATOM | 1067 | C | ILE | 132 | 15.954 | 49.155 | 112.508 | 1.00 | 10.16 | HIGL |
| ATOM | 1068 | O | ILE | 132 | 16.869 | 49.045 | 111.693 | 1.00 | 9.89 | HIGL |
| ATOM | 1069 | N | GLY | 133 | 16.160 | 49.253 | 113.814 | 1.00 | 9.99 | HIGL |
| ATOM | 1070 | CA | GLY | 133 | 17.500 | 49.230 | 114.364 | 1.00 | 10.91 | HIGL |
| ATOM | 1071 | C | GLY | 133 | 17.711 | 50.461 | 115.220 | 1.00 | 11.73 | HIGL |
| ATOM | 1072 | O | GLY | 133 | 16.885 | 51.378 | 115.193 | 1.00 | 11.22 | HIGL |
| ATOM | 1073 | N | ASN | 134 | 18.804 | 50.482 | 115.983 | 1.00 | 11.81 | HIGL |
| ATOM | 1074 | CA | ASN | 134 | 19.119 | 51.621 | 116.843 | 1.00 | 11.67 | HIGL |
| ATOM | 1075 | CB | ASN | 134 | 18.878 | 51.271 | 118.307 | 1.00 | 11.03 | HIGL |
| ATOM | 1076 | CG | ASN | 134 | 19.010 | 52.481 | 119.217 | 1.00 | 11.61 | HIGL |
| ATOM | 1077 | OD1 | ASN | 134 | 18.116 | 53.328 | 119.269 | 1.00 | 9.26 | HIGL |
| ATOM | 1078 | ND2 | ASN | 134 | 20.140 | 52.579 | 119.923 | 1.00 | 10.03 | HIGL |
| ATOM | 1079 | C | ASN | 134 | 20.578 | 52.041 | 116.673 | 1.00 | 12.23 | HIGL |
| ATOM | 1080 | O | ASN | 134 | 21.488 | 51.299 | 117.047 | 1.00 | 12.50 | HIGL |
| ATOM | 1081 | N | GLU | 135 | 20.796 | 53.237 | 116.130 | 1.00 | 12.34 | HIGL |
| ATOM | 1082 | CA | GLU | 135 | 22.148 | 53.745 | 115.905 | 1.00 | 12.34 | HIGL |
| ATOM | 1083 | CB | GLU | 135 | 22.819 | 54.137 | 117.233 | 1.00 | 12.86 | HIGL |
| ATOM | 1084 | CG | GLU | 135 | 22.107 | 55.229 | 118.021 | 1.00 | 13.57 | HIGL |
| ATOM | 1085 | CD | GLU | 135 | 22.988 | 55.855 | 119.109 | 1.00 | 14.70 | HIGL |
| ATOM | 1086 | OE1 | GLU | 135 | 23.605 | 55.107 | 119.895 | 1.00 | 13.98 | HIGL |
| ATOM | 1087 | OE2 | GLU | 135 | 23.059 | 57.100 | 119.186 | 1.00 | 14.17 | HIGL |
| ATOM | 1088 | C | GLU | 135 | 22.980 | 52.662 | 115.217 | 1.00 | 11.83 | HIGL |
| ATOM | 1089 | O | GLU | 135 | 24.062 | 52.307 | 115.689 | 1.00 | 11.40 | HIGL |
| ATOM | 1090 | N | ILE | 136 | 22.464 | 52.139 | 114.107 | 1.00 | 11.55 | HIGL |
| ATOM | 1091 | CA | ILE | 136 | 23.145 | 51.086 | 113.366 | 1.00 | 12.33 | HIGL |
| ATOM | 1092 | CB | ILE | 136 | 22.134 | 50.255 | 112.537 | 1.00 | 11.21 | HIGL |
| ATOM | 1093 | CG2 | ILE | 136 | 21.187 | 49.523 | 113.478 | 1.00 | 11.90 | HIGL |
| ATOM | 1094 | CG1 | ILE | 136 | 21.346 | 51.166 | 111.583 | 1.00 | 10.88 | HIGL |
| ATOM | 1095 | CD1 | ILE | 136 | 20.307 | 50.439 | 110.712 | 1.00 | 5.41 | HIGL |
| ATOM | 1096 | C | ILE | 136 | 24.272 | 51.570 | 112.446 | 1.00 | 13.31 | HIGL |
| ATOM | 1097 | O | ILE | 136 | 24.512 | 50.981 | 111.397 | 1.00 | 13.57 | HIGL |
| ATOM | 1098 | N | THR | 137 | 24.978 | 52.621 | 112.860 | 1.00 | 14.02 | HIGL |
| ATOM | 1099 | CA | THR | 137 | 26.076 | 53.177 | 112.073 | 1.00 | 15.42 | HIGL |
| ATOM | 1100 | CB | THR | 137 | 26.796 | 54.290 | 112.828 | 1.00 | 15.31 | HIGL |
| ATOM | 1101 | OG1 | THR | 137 | 25.835 | 55.190 | 113.390 | 1.00 | 15.48 | HIGL |
| ATOM | 1102 | CG2 | THR | 137 | 27.705 | 55.043 | 111.887 | 1.00 | 13.55 | HIGL |
| ATOM | 1103 | C | THR | 137 | 27.128 | 52.139 | 111.688 | 1.00 | 16.83 | HIGL |
| ATOM | 1104 | O | THR | 137 | 27.690 | 52.197 | 110.595 | 1.00 | 17.91 | HIGL |

# Fig. 2 cont.

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1105 | N | GLN | 138 | 27.421 | 51.214 | 112.596 | 1.00 | 17.23 | HIGL |
| ATOM | 1106 | CA | GLN | 138 | 28.396 | 50.166 | 112.308 | 1.00 | 17.23 | HIGL |
| ATOM | 1107 | CB | GLN | 138 | 29.328 | 49.926 | 113.503 | 1.00 | 18.55 | HIGL |
| ATOM | 1108 | CG | GLN | 138 | 30.240 | 51.101 | 113.856 | 1.00 | 22.06 | HIGL |
| ATOM | 1109 | CD | GLN | 138 | 30.963 | 51.687 | 112.642 | 1.00 | 24.27 | HIGL |
| ATOM | 1110 | OE1 | GLN | 138 | 31.641 | 50.975 | 111.897 | 1.00 | 24.26 | HIGL |
| ATOM | 1111 | NE2 | GLN | 138 | 30.821 | 52.997 | 112.445 | 1.00 | 24.87 | HIGL |
| ATOM | 1112 | C | GLN | 138 | 27.633 | 48.886 | 111.985 | 1.00 | 16.30 | HIGL |
| ATOM | 1113 | O | GLN | 138 | 28.133 | 47.774 | 112.187 | 1.00 | 15.80 | HIGL |
| ATOM | 1114 | N | GLY | 139 | 26.411 | 49.059 | 111.490 | 1.00 | 14.43 | HIGL |
| ATOM | 1115 | CA | GLY | 139 | 25.590 | 47.917 | 111.138 | 1.00 | 14.15 | HIGL |
| ATOM | 1116 | C | GLY | 139 | 24.778 | 47.376 | 112.304 | 1.00 | 13.48 | HIGL |
| ATOM | 1117 | O | GLY | 139 | 24.703 | 48.001 | 113.363 | 1.00 | 11.76 | HIGL |
| ATOM | 1118 | N | LEU | 140 | 24.175 | 46.207 | 112.098 | 1.00 | 12.77 | HIGL |
| ATOM | 1119 | CA | LEU | 140 | 23.353 | 45.562 | 113.114 | 1.00 | 12.79 | HIGL |
| ATOM | 1120 | CB | LEU | 140 | 21.878 | 45.922 | 112.917 | 1.00 | 12.46 | HIGL |
| ATOM | 1121 | CG | LEU | 140 | 21.162 | 45.335 | 111.695 | 1.00 | 12.85 | HIGL |
| ATOM | 1122 | CD1 | LEU | 140 | 19.672 | 45.582 | 111.817 | 1.00 | 13.35 | HIGL |
| ATOM | 1123 | CD2 | LEU | 140 | 21.687 | 45.954 | 110.416 | 1.00 | 12.87 | HIGL |
| ATOM | 1124 | C | LEU | 140 | 23.504 | 44.055 | 113.010 | 1.00 | 13.36 | HIGL |
| ATOM | 1125 | O | LEU | 140 | 24.120 | 43.554 | 112.072 | 1.00 | 13.25 | HIGL |
| ATOM | 1126 | N | LEU | 141 | 22.937 | 43.342 | 113.980 | 1.00 | 13.28 | HIGL |
| ATOM | 1127 | CA | LEU | 141 | 22.975 | 41.883 | 114.008 | 1.00 | 12.60 | HIGL |
| ATOM | 1128 | CB | LEU | 141 | 21.895 | 41.340 | 113.069 | 1.00 | 10.91 | HIGL |
| ATOM | 1129 | CG | LEU | 141 | 20.481 | 41.627 | 113.587 | 1.00 | 10.89 | HIGL |
| ATOM | 1130 | CD1 | LEU | 141 | 19.432 | 41.270 | 112.543 | 1.00 | 9.50 | HIGL |
| ATOM | 1131 | CD2 | LEU | 141 | 20.264 | 40.846 | 114.880 | 1.00 | 8.29 | HIGL |
| ATOM | 1132 | C | LEU | 141 | 24.337 | 41.284 | 113.656 | 1.00 | 13.21 | HIGL |
| ATOM | 1133 | O | LEU | 141 | 24.462 | 40.504 | 112.708 | 1.00 | 14.64 | HIGL |
| ATOM | 1134 | N | TRP | 142 | 25.353 | 41.644 | 114.432 | 1.00 | 13.26 | HIGL |
| ATOM | 1135 | CA | TRP | 142 | 26.705 | 41.149 | 114.204 | 1.00 | 13.14 | HIGL |
| ATOM | 1136 | CB | TRP | 142 | 27.686 | 41.859 | 115.130 | 1.00 | 11.33 | HIGL |
| ATOM | 1137 | CG | TRP | 142 | 27.757 | 43.330 | 114.910 | 1.00 | 10.90 | HIGL |
| ATOM | 1138 | CD2 | TRP | 142 | 28.488 | 44.272 | 115.695 | 1.00 | 11.10 | HIGL |
| ATOM | 1139 | CE2 | TRP | 142 | 28.289 | 45.545 | 115.113 | 1.00 | 11.19 | HIGL |
| ATOM | 1140 | CE3 | TRP | 142 | 29.290 | 44.167 | 116.835 | 1.00 | 10.40 | HIGL |
| ATOM | 1141 | CD1 | TRP | 142 | 27.158 | 44.046 | 113.911 | 1.00 | 10.69 | HIGL |
| ATOM | 1142 | NE1 | TRP | 142 | 27.474 | 45.379 | 114.025 | 1.00 | 10.00 | HIGL |
| ATOM | 1143 | CZ2 | TRP | 142 | 28.869 | 46.705 | 115.635 | 1.00 | 11.44 | HIGL |
| ATOM | 1144 | CZ3 | TRP | 142 | 29.863 | 45.319 | 117.353 | 1.00 | 11.67 | HIGL |
| ATOM | 1145 | CH2 | TRP | 142 | 29.650 | 46.573 | 116.750 | 1.00 | 11.55 | HIGL |
| ATOM | 1146 | C | TRP | 142 | 26.768 | 39.652 | 114.442 | 1.00 | 13.84 | HIGL |
| ATOM | 1147 | O | TRP | 142 | 26.046 | 39.126 | 115.286 | 1.00 | 14.95 | HIGL |
| ATOM | 1148 | N | PRO | 143 | 27.680 | 38.952 | 113.751 | 1.00 | 13.87 | HIGL |
| ATOM | 1149 | CD | PRO | 143 | 27.900 | 37.534 | 114.052 | 1.00 | 13.74 | HIGL |
| ATOM | 1150 | CA | PRO | 143 | 28.675 | 39.417 | 112.776 | 1.00 | 14.76 | HIGL |
| ATOM | 1151 | CB | PRO | 143 | 29.669 | 38.253 | 112.701 | 1.00 | 13.49 | HIGL |
| ATOM | 1152 | CG | PRO | 143 | 29.386 | 37.438 | 113.918 | 1.00 | 13.80 | HIGL |
| ATOM | 1153 | C | PRO | 143 | 28.174 | 39.778 | 111.381 | 1.00 | 15.67 | HIGL |
| ATOM | 1154 | O | PRO | 143 | 28.703 | 40.693 | 110.755 | 1.00 | 16.90 | HIGL |
| ATOM | 1155 | N | LEU | 144 | 27.182 | 39.044 | 110.887 | 1.00 | 15.74 | HIGL |
| ATOM | 1156 | CA | LEU | 144 | 26.648 | 39.272 | 109.549 | 1.00 | 16.05 | HIGL |
| ATOM | 1157 | CB | LEU | 144 | 25.366 | 38.459 | 109.358 | 1.00 | 15.16 | HIGL |
| ATOM | 1158 | CG | LEU | 144 | 25.558 | 36.942 | 109.467 | 1.00 | 14.79 | HIGL |
| ATOM | 1159 | CD1 | LEU | 144 | 24.214 | 36.248 | 109.414 | 1.00 | 14.16 | HIGL |
| ATOM | 1160 | CD2 | LEU | 144 | 26.455 | 36.449 | 108.331 | 1.00 | 14.04 | HIGL |
| ATOM | 1161 | C | LEU | 144 | 26.397 | 40.727 | 109.159 | 1.00 | 17.32 | HIGL |
| ATOM | 1162 | O | LEU | 144 | 26.911 | 41.191 | 108.144 | 1.00 | 17.71 | HIGL |
| ATOM | 1163 | N | GLY | 145 | 25.617 | 41.451 | 109.956 | 1.00 | 17.84 | HIGL |
| ATOM | 1164 | CA | GLY | 145 | 25.325 | 42.835 | 109.617 | 1.00 | 17.98 | HIGL |
| ATOM | 1165 | C | GLY | 145 | 26.335 | 43.888 | 110.051 | 1.00 | 18.71 | HIGL |
| ATOM | 1166 | O | GLY | 145 | 26.008 | 45.077 | 110.123 | 1.00 | 19.15 | HIGL |
| ATOM | 1167 | N | LYS | 146 | 27.560 | 43.477 | 110.341 | 1.00 | 18.29 | HIGL |
| ATOM | 1168 | CA | LYS | 146 | 28.575 | 44.428 | 110.762 | 1.00 | 19.30 | HIGL |
| ATOM | 1169 | CB | LYS | 146 | 29.733 | 43.687 | 111.423 | 1.00 | 18.95 | HIGL |

# Fig. 2 cont.

| ATOM | 1170 | CG | LYS | 146 | 30.533 | 44.508 | 112.414 | 1.00 | 18.69 | HIGL |
|------|------|-----|-----|-----|--------|--------|---------|------|-------|------|
| ATOM | 1171 | CD | LYS | 146 | 31.624 | 43.643 | 113.039 | 1.00 | 20.37 | HIGL |
| ATOM | 1172 | CE | LYS | 146 | 32.528 | 44.430 | 113.984 | 1.00 | 20.86 | HIGL |
| ATOM | 1173 | NZ | LYS | 146 | 31.799 | 44.955 | 115.162 | 1.00 | 21.63 | HIGL |
| ATOM | 1174 | C | LYS | 146 | 29.062 | 45.228 | 109.550 | 1.00 | 20.47 | HIGL |
| ATOM | 1175 | O | LYS | 146 | 29.211 | 44.685 | 108.453 | 1.00 | 19.27 | HIGL |
| ATOM | 1176 | N | THR | 147 | 29.312 | 46.519 | 109.752 | 1.00 | 21.74 | HIGL |
| ATOM | 1177 | CA | THR | 147 | 29.746 | 47.374 | 108.659 | 1.00 | 23.27 | HIGL |
| ATOM | 1178 | CB | THR | 147 | 30.212 | 48.734 | 109.130 | 1.00 | 22.61 | HIGL |
| ATOM | 1179 | OG1 | THR | 147 | 30.794 | 48.619 | 110.430 | 1.00 | 23.56 | HIGL |
| ATOM | 1180 | CG2 | THR | 147 | 29.050 | 49.703 | 109.127 | 1.00 | 23.05 | HIGL |
| ATOM | 1181 | C | THR | 147 | 30.817 | 46.833 | 107.747 | 1.00 | 24.76 | HIGL |
| ATOM | 1182 | O | THR | 147 | 31.763 | 46.161 | 108.173 | 1.00 | 24.27 | HIGL |
| ATOM | 1183 | N | ASN | 148 | 30.631 | 47.193 | 106.478 | 1.00 | 26.25 | HIGL |
| ATOM | 1184 | CA | ASN | 148 | 31.456 | 46.818 | 105.346 | 1.00 | 26.20 | HIGL |
| ATOM | 1185 | CB | ASN | 148 | 32.917 | 46.692 | 105.763 | 1.00 | 26.56 | HIGL |
| ATOM | 1186 | CG | ASN | 148 | 33.560 | 48.057 | 105.998 | 1.00 | 26.62 | HIGL |
| ATOM | 1187 | OD1 | ASN | 148 | 32.903 | 48.985 | 106.472 | 1.00 | 26.28 | HIGL |
| ATOM | 1188 | ND2 | ASN | 148 | 34.842 | 48.183 | 105.670 | 1.00 | 25.69 | HIGL |
| ATOM | 1189 | C | ASN | 148 | 30.865 | 45.542 | 104.762 | 1.00 | 26.28 | HIGL |
| ATOM | 1190 | O | ASN | 148 | 31.279 | 45.076 | 103.707 | 1.00 | 28.00 | HIGL |
| ATOM | 1191 | N | ASN | 149 | 29.873 | 44.998 | 105.464 | 1.00 | 25.38 | HIGL |
| ATOM | 1192 | CA | ASN | 149 | 29.127 | 43.826 | 105.007 | 1.00 | 24.20 | HIGL |
| ATOM | 1193 | CB | ASN | 149 | 28.733 | 42.927 | 106.177 | 1.00 | 24.04 | HIGL |
| ATOM | 1194 | CG | ASN | 149 | 29.858 | 42.016 | 106.615 | 1.00 | 24.57 | HIGL |
| ATOM | 1195 | OD1 | ASN | 149 | 31.033 | 42.309 | 106.391 | 1.00 | 25.70 | HIGL |
| ATOM | 1196 | ND2 | ASN | 149 | 29.505 | 40.910 | 107.260 | 1.00 | 23.86 | HIGL |
| ATOM | 1197 | C | ASN | 149 | 27.877 | 44.466 | 104.421 | 1.00 | 23.50 | HIGL |
| ATOM | 1198 | O | ASN | 149 | 26.753 | 44.012 | 104.637 | 1.00 | 24.05 | HIGL |
| ATOM | 1199 | N | TRP | 150 | 28.101 | 45.554 | 103.698 | 1.00 | 21.67 | HIGL |
| ATOM | 1200 | CA | TRP | 150 | 27.039 | 46.323 | 103.079 | 1.00 | 20.87 | HIGL |
| ATOM | 1201 | CB | TRP | 150 | 27.649 | 47.265 | 102.045 | 1.00 | 19.65 | HIGL |
| ATOM | 1202 | CG | TRP | 150 | 28.654 | 48.200 | 102.653 | 1.00 | 19.10 | HIGL |
| ATOM | 1203 | CD2 | TRP | 150 | 28.411 | 49.153 | 103.697 | 1.00 | 19.28 | HIGL |
| ATOM | 1204 | CE2 | TRP | 150 | 29.631 | 49.828 | 103.938 | 1.00 | 18.98 | HIGL |
| ATOM | 1205 | CE3 | TRP | 150 | 27.278 | 49.506 | 104.452 | 1.00 | 18.67 | HIGL |
| ATOM | 1206 | CD1 | TRP | 150 | 29.976 | 48.329 | 102.315 | 1.00 | 18.26 | HIGL |
| ATOM | 1207 | NE1 | TRP | 150 | 30.567 | 49.306 | 103.080 | 1.00 | 17.94 | HIGL |
| ATOM | 1208 | CZ2 | TRP | 150 | 29.751 | 50.837 | 104.902 | 1.00 | 19.36 | HIGL |
| ATOM | 1209 | CZ3 | TRP | 150 | 27.395 | 50.506 | 105.409 | 1.00 | 19.12 | HIGL |
| ATOM | 1210 | CH2 | TRP | 150 | 28.627 | 51.162 | 105.626 | 1.00 | 19.64 | HIGL |
| ATOM | 1211 | C | TRP | 150 | 25.939 | 45.479 | 102.451 | 1.00 | 20.95 | HIGL |
| ATOM | 1212 | O | TRP | 150 | 24.757 | 45.801 | 102.583 | 1.00 | 21.08 | HIGL |
| ATOM | 1213 | N | TYR | 151 | 26.315 | 44.400 | 101.769 | 1.00 | 20.56 | HIGL |
| ATOM | 1214 | CA | TYR | 151 | 25.312 | 43.551 | 101.146 | 1.00 | 19.67 | HIGL |
| ATOM | 1215 | CB | TYR | 151 | 25.949 | 42.403 | 100.362 | 1.00 | 19.65 | HIGL |
| ATOM | 1216 | CG | TYR | 151 | 24.910 | 41.515 | 99.711 | 1.00 | 20.60 | HIGL |
| ATOM | 1217 | CD1 | TYR | 151 | 24.183 | 41.962 | 98.610 | 1.00 | 20.83 | HIGL |
| ATOM | 1218 | CE1 | TYR | 151 | 23.180 | 41.179 | 98.036 | 1.00 | 20.50 | HIGL |
| ATOM | 1219 | CD2 | TYR | 151 | 24.609 | 40.249 | 100.228 | 1.00 | 20.51 | HIGL |
| ATOM | 1220 | CE2 | TYR | 151 | 23.601 | 39.457 | 99.656 | 1.00 | 20.06 | HIGL |
| ATOM | 1221 | CZ | TYR | 151 | 22.894 | 39.933 | 98.559 | 1.00 | 20.06 | HIGL |
| ATOM | 1222 | OH | TYR | 151 | 21.904 | 39.171 | 97.972 | 1.00 | 19.92 | HIGL |
| ATOM | 1223 | C | TYR | 151 | 24.389 | 42.972 | 102.204 | 1.00 | 19.26 | HIGL |
| ATOM | 1224 | O | TYR | 151 | 23.176 | 43.114 | 102.113 | 1.00 | 18.33 | HIGL |
| ATOM | 1225 | N | ASN | 152 | 24.966 | 42.317 | 103.209 | 1.00 | 19.42 | HIGL |
| ATOM | 1226 | CA | ASN | 152 | 24.158 | 41.722 | 104.267 | 1.00 | 19.11 | HIGL |
| ATOM | 1227 | CB | ASN | 152 | 25.040 | 41.046 | 105.326 | 1.00 | 19.23 | HIGL |
| ATOM | 1228 | CG | ASN | 152 | 25.663 | 39.739 | 104.835 | 1.00 | 20.56 | HIGL |
| ATOM | 1229 | OD1 | ASN | 152 | 25.221 | 39.154 | 103.839 | 1.00 | 19.15 | HIGL |
| ATOM | 1230 | ND2 | ASN | 152 | 26.687 | 39.267 | 105.549 | 1.00 | 19.90 | HIGL |
| ATOM | 1231 | C | ASN | 152 | 23.265 | 42.756 | 104.937 | 1.00 | 18.86 | HIGL |
| ATOM | 1232 | O | ASN | 152 | 22.111 | 42.469 | 105.248 | 1.00 | 19.25 | HIGL |
| ATOM | 1233 | N | ILE | 153 | 23.792 | 43.958 | 105.154 | 1.00 | 18.55 | HIGL |
| ATOM | 1234 | CA | ILE | 153 | 23.024 | 45.020 | 105.804 | 1.00 | 18.75 | HIGL |

# Fig. 2 cont.

| ATOM | 1235 | CB   | ILE | 153 | 23.891 | 46.283 | 106.033 | 1.00 | 17.77 | HIGL |
|------|------|------|-----|-----|--------|--------|---------|------|-------|------|
| ATOM | 1236 | CG2  | ILE | 153 | 23.053 | 47.395 | 106.623 | 1.00 | 16.52 | HIGL |
| ATOM | 1237 | CG1  | ILE | 153 | 25.046 | 45.949 | 106.982 | 1.00 | 17.36 | HIGL |
| ATOM | 1238 | CD1  | ILE | 153 | 26.068 | 47.050 | 107.128 | 1.00 | 16.15 | HIGL |
| ATOM | 1239 | C    | ILE | 153 | 21.770 | 45.414 | 105.021 | 1.00 | 19.29 | HIGL |
| ATOM | 1240 | O    | ILE | 153 | 20.653 | 45.369 | 105.557 | 1.00 | 18.88 | HIGL |
| ATOM | 1241 | N    | ALA | 154 | 21.950 | 45.791 | 103.758 | 1.00 | 18.63 | HIGL |
| ATOM | 1242 | CA   | ALA | 154 | 20.814 | 46.198 | 102.936 | 1.00 | 19.02 | HIGL |
| ATOM | 1243 | CB   | ALA | 154 | 21.280 | 46.567 | 101.536 | 1.00 | 17.23 | HIGL |
| ATOM | 1244 | C    | ALA | 154 | 19.828 | 45.043 | 102.880 | 1.00 | 19.18 | HIGL |
| ATOM | 1245 | O    | ALA | 154 | 18.609 | 45.227 | 102.823 | 1.00 | 19.09 | HIGL |
| ATOM | 1246 | N    | ARG | 155 | 20.393 | 43.846 | 102.908 | 1.00 | 19.15 | HIGL |
| ATOM | 1247 | CA   | ARG | 155 | 19.646 | 42.602 | 102.864 | 1.00 | 18.74 | HIGL |
| ATOM | 1248 | CB   | ARG | 155 | 20.661 | 41.461 | 102.775 | 1.00 | 18.99 | HIGL |
| ATOM | 1249 | CG   | ARG | 155 | 20.110 | 40.111 | 102.485 | 1.00 | 19.95 | HIGL |
| ATOM | 1250 | CD   | ARG | 155 | 19.495 | 39.997 | 101.104 | 1.00 | 20.00 | HIGL |
| ATOM | 1251 | NE   | ARG | 155 | 18.768 | 38.740 | 101.065 | 1.00 | 21.33 | HIGL |
| ATOM | 1252 | CZ   | ARG | 155 | 19.341 | 37.554 | 100.901 | 1.00 | 22.66 | HIGL |
| ATOM | 1253 | NH1  | ARG | 155 | 20.655 | 37.462 | 100.728 | 1.00 | 22.62 | HIGL |
| ATOM | 1254 | NH2  | ARG | 155 | 18.607 | 36.454 | 100.981 | 1.00 | 24.41 | HIGL |
| ATOM | 1255 | C    | ARG | 155 | 18.798 | 42.509 | 104.142 | 1.00 | 18.62 | HIGL |
| ATOM | 1256 | O    | ARG | 155 | 17.593 | 42.257 | 104.105 | 1.00 | 18.01 | HIGL |
| ATOM | 1257 | N    | LEU | 156 | 19.432 | 42.748 | 105.280 | 1.00 | 18.71 | HIGL |
| ATOM | 1258 | CA   | LEU | 156 | 18.725 | 42.688 | 106.548 | 1.00 | 17.91 | HIGL |
| ATOM | 1259 | CB   | LEU | 156 | 19.720 | 42.796 | 107.707 | 1.00 | 16.34 | HIGL |
| ATOM | 1260 | CG   | LEU | 156 | 20.507 | 41.507 | 107.927 | 1.00 | 16.27 | HIGL |
| ATOM | 1261 | CD1  | LEU | 156 | 21.555 | 41.716 | 109.000 | 1.00 | 15.19 | HIGL |
| ATOM | 1262 | CD2  | LEU | 156 | 19.547 | 40.384 | 108.310 | 1.00 | 15.70 | HIGL |
| ATOM | 1263 | C    | LEU | 156 | 17.651 | 43.757 | 106.680 | 1.00 | 17.08 | HIGL |
| ATOM | 1264 | O    | LEU | 156 | 16.531 | 43.472 | 107.097 | 1.00 | 18.08 | HIGL |
| ATOM | 1265 | N    | LEU | 157 | 17.984 | 44.987 | 106.323 | 1.00 | 16.61 | HIGL |
| ATOM | 1266 | CA   | LEU | 157 | 17.025 | 46.069 | 106.448 | 1.00 | 16.27 | HIGL |
| ATOM | 1267 | CB   | LEU | 157 | 17.710 | 47.405 | 106.169 | 1.00 | 15.39 | HIGL |
| ATOM | 1268 | CG   | LEU | 157 | 18.901 | 47.674 | 107.103 | 1.00 | 15.27 | HIGL |
| ATOM | 1269 | CD1  | LEU | 157 | 19.582 | 48.989 | 106.730 | 1.00 | 14.68 | HIGL |
| ATOM | 1270 | CD2  | LEU | 157 | 18.425 | 47.688 | 108.546 | 1.00 | 13.43 | HIGL |
| ATOM | 1271 | C    | LEU | 157 | 15.819 | 45.870 | 105.543 | 1.00 | 16.79 | HIGL |
| ATOM | 1272 | O    | LEU | 157 | 14.686 | 46.120 | 105.950 | 1.00 | 17.48 | HIGL |
| ATOM | 1273 | N    | HIS | 158 | 16.050 | 45.403 | 104.321 | 1.00 | 17.58 | HIGL |
| ATOM | 1274 | CA   | HIS | 158 | 14.944 | 45.174 | 103.401 | 1.00 | 17.25 | HIGL |
| ATOM | 1275 | CB   | HIS | 158 | 15.439 | 44.552 | 102.099 | 1.00 | 17.36 | HIGL |
| ATOM | 1276 | CG   | HIS | 158 | 14.335 | 44.187 | 101.159 | 1.00 | 18.88 | HIGL |
| ATOM | 1277 | CD2  | HIS | 158 | 13.798 | 42.986 | 100.834 | 1.00 | 18.45 | HIGL |
| ATOM | 1278 | ND1  | HIS | 158 | 13.587 | 45.133 | 100.484 | 1.00 | 19.56 | HIGL |
| ATOM | 1279 | CE1  | HIS | 158 | 12.641 | 44.530 | 99.790  | 1.00 | 18.81 | HIGL |
| ATOM | 1280 | NE2  | HIS | 158 | 12.746 | 43.225 | 99.985  | 1.00 | 19.02 | HIGL |
| ATOM | 1281 | C    | HIS | 158 | 13.920 | 44.242 | 104.051 | 1.00 | 17.47 | HIGL |
| ATOM | 1282 | O    | HIS | 158 | 12.723 | 44.531 | 104.066 | 1.00 | 16.46 | HIGL |
| ATOM | 1283 | N    | SER | 159 | 14.402 | 43.127 | 104.592 | 1.00 | 17.53 | HIGL |
| ATOM | 1284 | CA   | SER | 159 | 13.535 | 42.157 | 105.244 | 1.00 | 17.96 | HIGL |
| ATOM | 1285 | CB   | SER | 159 | 14.353 | 40.973 | 105.753 | 1.00 | 18.70 | HIGL |
| ATOM | 1286 | OG   | SER | 159 | 14.963 | 40.280 | 104.684 | 1.00 | 20.45 | HIGL |
| ATOM | 1287 | C    | SER | 159 | 12.778 | 42.782 | 106.409 | 1.00 | 18.11 | HIGL |
| ATOM | 1288 | O    | SER | 159 | 11.577 | 42.549 | 106.577 | 1.00 | 17.79 | HIGL |
| ATOM | 1289 | N    | ALA | 160 | 13.483 | 43.573 | 107.214 | 1.00 | 17.67 | HIGL |
| ATOM | 1290 | CA   | ALA | 160 | 12.871 | 44.231 | 108.363 | 1.00 | 17.44 | HIGL |
| ATOM | 1291 | CB   | ALA | 160 | 13.929 | 44.922 | 109.187 | 1.00 | 16.81 | HIGL |
| ATOM | 1292 | C    | ALA | 160 | 11.824 | 45.239 | 107.918 | 1.00 | 17.59 | HIGL |
| ATOM | 1293 | O    | ALA | 160 | 10.737 | 45.322 | 108.492 | 1.00 | 17.41 | HIGL |
| ATOM | 1294 | N    | ALA | 161 | 12.157 | 46.012 | 106.892 | 1.00 | 18.14 | HIGL |
| ATOM | 1295 | CA   | ALA | 161 | 11.230 | 47.011 | 106.377 | 1.00 | 18.38 | HIGL |
| ATOM | 1296 | CB   | ALA | 161 | 11.831 | 47.714 | 105.189 | 1.00 | 16.08 | HIGL |
| ATOM | 1297 | C    | ALA | 161 | 9.931  | 46.337 | 105.974 | 1.00 | 19.43 | HIGL |
| ATOM | 1298 | O    | ALA | 161 | 8.844  | 46.848 | 106.244 | 1.00 | 20.06 | HIGL |
| ATOM | 1299 | N    | TRP | 162 | 10.045 | 45.176 | 105.335 | 1.00 | 19.98 | HIGL |

# Fig. 2 cont.

| ATOM | 1300 | CA  | TRP | 162 | 8.864  | 44.463 | 104.889 | 1.00 | 20.45 | HIGL |
|------|------|-----|-----|-----|--------|--------|---------|------|-------|------|
| ATOM | 1301 | CB  | TRP | 162 | 9.215  | 43.511 | 103.746 | 1.00 | 21.00 | HIGL |
| ATOM | 1302 | CG  | TRP | 162 | 9.298  | 44.267 | 102.482 | 1.00 | 21.58 | HIGL |
| ATOM | 1303 | CD2 | TRP | 162 | 8.222  | 44.516 | 101.575 | 1.00 | 21.96 | HIGL |
| ATOM | 1304 | CE2 | TRP | 162 | 8.691  | 45.440 | 100.612 | 1.00 | 21.86 | HIGL |
| ATOM | 1305 | CE3 | TRP | 162 | 6.902  | 44.056 | 101.487 | 1.00 | 22.03 | HIGL |
| ATOM | 1306 | CD1 | TRP | 162 | 10.354 | 45.019 | 102.040 | 1.00 | 21.86 | HIGL |
| ATOM | 1307 | NE1 | TRP | 162 | 9.995  | 45.729 | 100.919 | 1.00 | 21.88 | HIGL |
| ATOM | 1308 | CZ2 | TRP | 162 | 7.884  | 45.913 | 99.572  | 1.00 | 21.45 | HIGL |
| ATOM | 1309 | CZ3 | TRP | 162 | 6.096  | 44.530 | 100.448 | 1.00 | 22.27 | HIGL |
| ATOM | 1310 | CH2 | TRP | 162 | 6.594  | 45.449 | 99.506  | 1.00 | 21.62 | HIGL |
| ATOM | 1311 | C   | TRP | 162 | 8.108  | 43.746 | 105.982 | 1.00 | 20.46 | HIGL |
| ATOM | 1312 | O   | TRP | 162 | 6.919  | 43.463 | 105.829 | 1.00 | 21.30 | HIGL |
| ATOM | 1313 | N   | GLY | 163 | 8.783  | 43.453 | 107.085 | 1.00 | 19.69 | HIGL |
| ATOM | 1314 | CA  | GLY | 163 | 8.089  | 42.816 | 108.182 | 1.00 | 19.99 | HIGL |
| ATOM | 1315 | C   | GLY | 163 | 7.048  | 43.833 | 108.622 | 1.00 | 20.35 | HIGL |
| ATOM | 1316 | O   | GLY | 163 | 5.954  | 43.491 | 109.075 | 1.00 | 20.66 | HIGL |
| ATOM | 1317 | N   | VAL | 164 | 7.398  | 45.106 | 108.469 | 1.00 | 19.87 | HIGL |
| ATOM | 1318 | CA  | VAL | 164 | 6.504  | 46.194 | 108.832 | 1.00 | 18.68 | HIGL |
| ATOM | 1319 | CB  | VAL | 164 | 7.266  | 47.534 | 108.946 | 1.00 | 18.24 | HIGL |
| ATOM | 1320 | CG1 | VAL | 164 | 6.305  | 48.650 | 109.336 | 1.00 | 17.70 | HIGL |
| ATOM | 1321 | CG2 | VAL | 164 | 8.391  | 47.409 | 109.959 | 1.00 | 17.30 | HIGL |
| ATOM | 1322 | C   | VAL | 164 | 5.447  | 46.336 | 107.748 | 1.00 | 18.61 | HIGL |
| ATOM | 1323 | O   | VAL | 164 | 4.254  | 46.415 | 108.027 | 1.00 | 18.31 | HIGL |
| ATOM | 1324 | N   | LYS | 165 | 5.891  | 46.356 | 106.502 | 1.00 | 18.63 | HIGL |
| ATOM | 1325 | CA  | LYS | 165 | 4.965  | 46.516 | 105.403 | 1.00 | 19.93 | HIGL |
| ATOM | 1326 | CB  | LYS | 165 | 5.728  | 46.615 | 104.087 | 1.00 | 19.36 | HIGL |
| ATOM | 1327 | CG  | LYS | 165 | 6.589  | 47.869 | 103.981 | 1.00 | 18.36 | HIGL |
| ATOM | 1328 | CD  | LYS | 165 | 7.335  | 47.923 | 102.644 | 1.00 | 18.25 | HIGL |
| ATOM | 1329 | CE  | LYS | 165 | 8.175  | 49.182 | 102.534 | 1.00 | 17.76 | HIGL |
| ATOM | 1330 | NZ  | LYS | 165 | 7.317  | 50.401 | 102.629 | 1.00 | 18.31 | HIGL |
| ATOM | 1331 | C   | LYS | 165 | 3.904  | 45.428 | 105.325 | 1.00 | 20.82 | HIGL |
| ATOM | 1332 | O   | LYS | 165 | 2.746  | 45.727 | 105.049 | 1.00 | 21.60 | HIGL |
| ATOM | 1333 | N   | ASP | 166 | 4.283  | 44.179 | 105.581 | 1.00 | 21.39 | HIGL |
| ATOM | 1334 | CA  | ASP | 166 | 3.327  | 43.073 | 105.522 | 1.00 | 22.03 | HIGL |
| ATOM | 1335 | CB  | ASP | 166 | 4.039  | 41.749 | 105.219 | 1.00 | 22.56 | HIGL |
| ATOM | 1336 | CG  | ASP | 166 | 4.642  | 41.702 | 103.833 | 1.00 | 23.22 | HIGL |
| ATOM | 1337 | OD1 | ASP | 166 | 4.195  | 42.463 | 102.951 | 1.00 | 23.72 | HIGL |
| ATOM | 1338 | OD2 | ASP | 166 | 5.560  | 40.879 | 103.623 | 1.00 | 23.83 | HIGL |
| ATOM | 1339 | C   | ASP | 166 | 2.481  | 42.860 | 106.782 | 1.00 | 22.48 | HIGL |
| ATOM | 1340 | O   | ASP | 166 | 1.724  | 41.896 | 106.852 | 1.00 | 22.92 | HIGL |
| ATOM | 1341 | N   | SER | 167 | 2.596  | 43.732 | 107.777 | 1.00 | 22.71 | HIGL |
| ATOM | 1342 | CA  | SER | 167 | 1.825  | 43.554 | 109.006 | 1.00 | 22.64 | HIGL |
| ATOM | 1343 | CB  | SER | 167 | 2.519  | 44.259 | 110.169 | 1.00 | 22.61 | HIGL |
| ATOM | 1344 | OG  | SER | 167 | 2.442  | 45.667 | 110.023 | 1.00 | 23.18 | HIGL |
| ATOM | 1345 | C   | SER | 167 | 0.396  | 44.081 | 108.886 | 1.00 | 23.16 | HIGL |
| ATOM | 1346 | O   | SER | 167 | 0.040  | 44.722 | 107.903 | 1.00 | 22.85 | HIGL |
| ATOM | 1347 | N   | ARG | 168 | -0.418 | 43.798 | 109.898 | 1.00 | 23.80 | HIGL |
| ATOM | 1348 | CA  | ARG | 168 | -1.805 | 44.250 | 109.933 | 1.00 | 23.78 | HIGL |
| ATOM | 1349 | CB  | ARG | 168 | -2.601 | 43.465 | 110.978 | 1.00 | 23.09 | HIGL |
| ATOM | 1350 | CG  | ARG | 168 | -3.597 | 42.463 | 110.420 | 1.00 | 22.15 | HIGL |
| ATOM | 1351 | CD  | ARG | 168 | -3.088 | 41.049 | 110.571 | 1.00 | 21.65 | HIGL |
| ATOM | 1352 | NE  | ARG | 168 | -2.910 | 40.664 | 111.971 | 1.00 | 18.91 | HIGL |
| ATOM | 1353 | CZ  | ARG | 168 | -2.272 | 39.564 | 112.348 | 1.00 | 18.78 | HIGL |
| ATOM | 1354 | NH1 | ARG | 168 | -1.763 | 38.753 | 111.430 | 1.00 | 18.16 | HIGL |
| ATOM | 1355 | NH2 | ARG | 168 | -2.127 | 39.278 | 113.633 | 1.00 | 19.17 | HIGL |
| ATOM | 1356 | C   | ARG | 168 | -1.890 | 45.734 | 110.284 | 1.00 | 24.65 | HIGL |
| ATOM | 1357 | O   | ARG | 168 | -2.980 | 46.299 | 110.348 | 1.00 | 25.72 | HIGL |
| ATOM | 1358 | N   | LEU | 169 | -0.751 | 46.366 | 110.534 | 1.00 | 24.93 | HIGL |
| ATOM | 1359 | CA  | LEU | 169 | -0.767 | 47.779 | 110.873 | 1.00 | 25.57 | HIGL |
| ATOM | 1360 | CB  | LEU | 169 | 0.642  | 48.300 | 111.135 | 1.00 | 24.39 | HIGL |
| ATOM | 1361 | CG  | LEU | 169 | 1.239  | 47.981 | 112.501 | 1.00 | 23.91 | HIGL |
| ATOM | 1362 | CD1 | LEU | 169 | 2.643  | 48.570 | 112.579 | 1.00 | 23.28 | HIGL |
| ATOM | 1363 | CD2 | LEU | 169 | 0.350  | 48.545 | 113.595 | 1.00 | 21.07 | HIGL |
| ATOM | 1364 | C   | LEU | 169 | -1.395 | 48.596 | 109.768 | 1.00 | 26.78 | HIGL |

# Fig. 2 cont.

| ATOM | 1365 | O   | LEU | 169  | -1.086 | 48.421 | 108.591 | 1.00 | 26.61 | HIGL |
|------|------|-----|-----|------|--------|--------|---------|------|-------|------|
| ATOM | 1366 | N   | ASN | 170  | -2.292 | 49.485 | 110.160 | 1.00 | 28.98 | HIGL |
| ATOM | 1367 | CA  | ASN | 170  | -2.962 | 50.356 | 109.216 | 1.00 | 31.16 | HIGL |
| ATOM | 1368 | CB  | ASN | 170  | -4.126 | 49.638 | 108.536 | 1.00 | 34.31 | HIGL |
| ATOM | 1369 | CG  | ASN | 170  | -4.532 | 50.301 | 107.223 | 1.00 | 37.73 | HIGL |
| ATOM | 1370 | OD1 | ASN | 170  | -5.637 | 50.087 | 106.717 | 1.00 | 39.55 | HIGL |
| ATOM | 1371 | ND2 | ASN | 170  | -3.628 | 51.098 | 106.657 | 1.00 | 38.83 | HIGL |
| ATOM | 1372 | C   | ASN | 170  | -3.482 | 51.560 | 109.989 | 1.00 | 31.18 | HIGL |
| ATOM | 1373 | O   | ASN | 170  | -4.227 | 51.411 | 110.965 | 1.00 | 31.87 | HIGL |
| ATOM | 1374 | N   | PRO | 171  | -3.044 | 52.767 | 109.599 | 1.00 | 29.94 | HIGL |
| ATOM | 1375 | CD  | PRO | 171  | -3.373 | 54.060 | 110.227 | 1.00 | 29.80 | HIGL |
| ATOM | 1376 | CA  | PRO | 171  | -2.101 | 52.949 | 108.492 | 1.00 | 28.18 | HIGL |
| ATOM | 1377 | CB  | PRO | 171  | -2.094 | 54.459 | 108.295 | 1.00 | 28.38 | HIGL |
| ATOM | 1378 | CG  | PRO | 171  | -2.269 | 54.960 | 109.698 | 1.00 | 29.83 | HIGL |
| ATOM | 1379 | C   | PRO | 171  | -0.728 | 52.413 | 108.889 | 1.00 | 26.71 | HIGL |
| ATOM | 1380 | O   | PRO | 171  | -0.472 | 52.183 | 110.068 | 1.00 | 25.16 | HIGL |
| ATOM | 1381 | N   | LYS | 172  | 0.139  | 52.204 | 107.900 | 1.00 | 25.19 | HIGL |
| ATOM | 1382 | CA  | LYS | 172  | 1.482  | 51.709 | 108.155 | 1.00 | 24.35 | HIGL |
| ATOM | 1383 | CB  | LYS | 172  | 2.119  | 51.187 | 106.867 | 1.00 | 25.60 | HIGL |
| ATOM | 1384 | CG  | LYS | 172  | 1.274  | 50.201 | 106.093 | 1.00 | 27.94 | HIGL |
| ATOM | 1385 | CD  | LYS | 172  | 1.253  | 48.826 | 106.725 | 1.00 | 29.37 | HIGL |
| ATOM | 1386 | CE  | LYS | 172  | 0.451  | 47.875 | 105.848 | 1.00 | 30.03 | HIGL |
| ATOM | 1387 | NZ  | LYS | 172  | 0.492  | 46.469 | 106.329 | 1.00 | 30.93 | HIGL |
| ATOM | 1388 | C   | LYS | 172  | 2.332  | 52.858 | 108.686 | 1.00 | 22.94 | HIGL |
| ATOM | 1389 | O   | LYS | 172  | 2.212  | 53.992 | 108.220 | 1.00 | 22.83 | HIGL |
| ATOM | 1390 | N   | PRO | 173  | 3.200  | 52.580 | 109.671 | 1.00 | 21.18 | HIGL |
| ATOM | 1391 | CD  | PRO | 173  | 3.396  | 51.290 | 110.354 | 1.00 | 21.36 | HIGL |
| ATOM | 1392 | CA  | PRO | 173· | 4.069  | 53.599 | 110.254 | 1.00 | 20.28 | HIGL |
| ATOM | 1393 | CB  | PRO | 173  | 4.595  | 52.915 | 111.508 | 1.00 | 20.26 | HIGL |
| ATOM | 1394 | CG  | PRO | 173  | 4.718  | 51.502 | 111.059 | 1.00 | 20.58 | HIGL |
| ATOM | 1395 | C   | PRO | 173  | 5.197  | 53.947 | 109.297 | 1.00 | 19.51 | HIGL |
| ATOM | 1396 | O   | PRO | 173  | 5.525  | 53.172 | 108.407 | 1.00 | 19.40 | HIGL |
| ATOM | 1397 | N   | LYS | 174  | 5.778  | 55.123 | 109.482 | 1.00 | 18.84 | HIGL |
| ATOM | 1398 | CA  | LYS | 174  | 6.887  | 55.548 | 108.655 | 1.00 | 18.05 | HIGL |
| ATOM | 1399 | CB  | LYS | 174  | 7.168  | 57.032 | 108.875 | 1.00 | 18.15 | HIGL |
| ATOM | 1400 | CG  | LYS | 174  | 5.984  | 57.905 | 108.527 | 1.00 | 18.80 | HIGL |
| ATOM | 1401 | CD  | LYS | 174  | 6.308  | 59.380 | 108.602 | 1.00 | 19.52 | HIGL |
| ATOM | 1402 | CE  | LYS | 174  | 5.140  | 60.200 | 108.085 | 1.00 | 18.38 | HIGL |
| ATOM | 1403 | NZ  | LYS | 174  | 5.521  | 61.622 | 107.893 | 1.00 | 19.70 | HIGL |
| ATOM | 1404 | C   | LYS | 174  | 8.073  | 54.712 | 109.097 | 1.00 | 17.68 | HIGL |
| ATOM | 1405 | O   | LYS | 174  | 8.348  | 54.586 | 110.288 | 1.00 | 18.33 | HIGL |
| ATOM | 1406 | N   | ILE | 175  | 8.764  | 54.119 | 108.139 | 1.00 | 17.03 | HIGL |
| ATOM | 1407 | CA  | ILE | 175  | 9.·909 | 53.291 | 108.461 | 1.00 | 16.37 | HIGL |
| ATOM | 1408 | CB  | ILE | 175  | 10.071 | 52.178 | 107.420 | 1.00 | 15.88 | HIGL |
| ATOM | 1409 | CG2 | ILE | 175  | 11.276 | 51.317 | 107.767 | 1.00 | 14.85 | HIGL |
| ATOM | 1410 | CG1 | ILE | 175· | 8.785  | 51.342 | 107.387 | 1.00 | 14.92 | HIGL |
| ATOM | 1411 | CD1 | ILE | 175  | 8.694  | 50.358 | 106.232 | 1.00 | 16.47 | HIGL |
| ATOM | 1412 | C   | ILE | 175  | 11.142 | 54.176 | 108.517 | 1.00 | 15.73 | HIGL |
| ATOM | 1413 | O   | ILE | 175  | 11.417 | 54.933 | 107.588 | 1.00 | 15.78 | HIGL |
| ATOM | 1414 | N   | MET | 176  | 11.874 | 54.075 | 109.620 | 1.00 | 14.73 | HIGL |
| ATOM | 1415 | CA  | MET | 176  | 13.054 | 54.896 | 109.836 | 1.00 | 14.35 | HIGL |
| ATOM | 1416 | CB  | MET | 176  | 12.830 | 55.786 | 111.070 | 1.00 | 13.52 | HIGL |
| ATOM | 1417 | CG  | MET | 176  | 14.060 | 56.557 | 111.518 | 1.00 | 13.16 | HIGL |
| ATOM | 1418 | SD  | MET | 176  | 13.928 | 57.167 | 113.201 | 1.00 | 14.72 | HIGL |
| ATOM | 1419 | CE  | MET | 176  | 12.695 | 58.477 | 112.999 | 1.00 | 14.08 | HIGL |
| ATOM | 1420 | C   | MET | 176  | 14.358 | 54.122 | 110.024 | 1.00 | 14.18 | HIGL |
| ATOM | 1421 | O   | MET | 176  | 14.376 | 53.040 | 110.603 | 1.00 | 14.19 | HIGL |
| ATOM | 1422 | N   | VAL | 177  | 15.444 | 54.693 | 109.511 | 1.00 | 14.60 | HIGL |
| ATOM | 1423 | CA  | VAL | 177  | 16.777 | 54.123 | 109.664 | 1.00 | 13.89 | HIGL |
| ATOM | 1424 | CB  | VAL | 177  | 17.532 | 54.024 | 108.319 | 1.00 | 13.58 | HIGL |
| ATOM | 1425 | CG1 | VAL | 177  | 19.004 | 53.680 | 108.573 | 1.00 | 12.32 | HIGL |
| ATOM | 1426 | CG2 | VAL | 177  | 16.892 | 52.940 | 107.454 | 1.00 | 12.15 | HIGL |
| ATOM | 1427 | C   | VAL | 177  | 17.461 | 55.113 | 110.597 | 1.00 | 13.92 | HIGL |
| ATOM | 1428 | O   | VAL | 177  | 17.503 | 56.314 | 110.326 | 1.00 | 13.57 | HIGL |
| ATOM | 1429 | N   | HIS | 178  | 17.966 | 54.595 | 111.710 | 1.00 | 14.28 | HIGL |

# Fig. 2 cont.

| ATOM | 1430 | CA  | HIS | 178 | 18.591 | 55.407 | 112.743 | 1.00 | 14.37 | HIGL |
|------|------|-----|-----|-----|--------|--------|---------|------|-------|------|
| ATOM | 1431 | CB  | HIS | 178 | 17.910 | 55.083 | 114.083 | 1.00 | 14.38 | HIGL |
| ATOM | 1432 | CG  | HIS | 178 | 18.522 | 55.762 | 115.268 | 1.00 | 14.85 | HIGL |
| ATOM | 1433 | CD2 | HIS | 178 | 18.456 | 55.471 | 116.589 | 1.00 | 14.94 | HIGL |
| ATOM | 1434 | ND1 | HIS | 178 | 19.287 | 56.903 | 115.163 | 1.00 | 15.06 | HIGL |
| ATOM | 1435 | CE1 | HIS | 178 | 19.670 | 57.285 | 116.369 | 1.00 | 14.39 | HIGL |
| ATOM | 1436 | NE2 | HIS | 178 | 19.179 | 56.434 | 117.251 | 1.00 | 15.19 | HIGL |
| ATOM | 1437 | C   | HIS | 178 | 20.102 | 55.235 | 112.850 | 1.00 | 14.74 | HIGL |
| ATOM | 1438 | O   | HIS | 178 | 20.605 | 54.132 | 113.072 | 1.00 | 14.60 | HIGL |
| ATOM | 1439 | N   | LEU | 179 | 20.812 | 56.346 | 112.685 | 1.00 | 14.68 | HIGL |
| ATOM | 1440 | CA  | LEU | 179 | 22.269 | 56.381 | 112.769 | 1.00 | 14.88 | HIGL |
| ATOM | 1441 | CB  | LEU | 179 | 22.866 | 56.817 | 111.430 | 1.00 | 14.85 | HIGL |
| ATOM | 1442 | CG  | LEU | 179 | 23.217 | 55.794 | 110.349 | 1.00 | 15.01 | HIGL |
| ATOM | 1443 | CD1 | LEU | 179 | 22.120 | 54.786 | 110.177 | 1.00 | 15.16 | HIGL |
| ATOM | 1444 | CD2 | LEU | 179 | 23.476 | 56.536 | 109.049 | 1.00 | 14.52 | HIGL |
| ATOM | 1445 | C   | LEU | 179 | 22.632 | 57.406 | 113.830 | 1.00 | 14.77 | HIGL |
| ATOM | 1446 | O   | LEU | 179 | 21.867 | 58.336 | 114.070 | 1.00 | 16.15 | HIGL |
| ATOM | 1447 | N   | ASP | 180 | 23.786 | 57.244 | 114.468 | 1.00 | 14.56 | HIGL |
| ATOM | 1448 | CA  | ASP | 180 | 24.217 | 58.200 | 115.483 | 1.00 | 15.13 | HIGL |
| ATOM | 1449 | CB  | ASP | 180 | 25.040 | 57.491 | 116.576 | 1.00 | 15.21 | HIGL |
| ATOM | 1450 | CG  | ASP | 180 | 26.496 | 57.238 | 116.171 | 1.00 | 16.64 | HIGL |
| ATOM | 1451 | OD1 | ASP | 180 | 26.744 | 56.712 | 115.060 | 1.00 | 15.02 | HIGL |
| ATOM | 1452 | OD2 | ASP | 180 | 27.393 | 57.560 | 116.987 | 1.00 | 16.16 | HIGL |
| ATOM | 1453 | C   | ASP | 180 | 25.039 | 59.279 | 114.776 | 1.00 | 15.95 | HIGL |
| ATOM | 1454 | O   | ASP | 180 | 25.185 | 59.233 | 113.555 | 1.00 | 17.25 | HIGL |
| ATOM | 1455 | N   | ASN | 181 | 25.556 | 60.249 | 115.525 | 1.00 | 15.91 | HIGL |
| ATOM | 1456 | CA  | ASN | 181 | 26.362 | 61.334 | 114.960 | 1.00 | 15.67 | HIGL |
| ATOM | 1457 | CB  | ASN | 181 | 27.754 | 60.824 | 114.594 | 1.00 | 16.57 | HIGL |
| ATOM | 1458 | CG  | ASN | 181 | 28.573 | 60.449 | 115.807 | 1.00 | 17.66 | HIGL |
| ATOM | 1459 | OD1 | ASN | 181 | 28.418 | 61.031 | 116.881 | 1.00 | 19.18 | HIGL |
| ATOM | 1460 | ND2 | ASN | 181 | 29.464 | 59.487 | 115.641 | 1.00 | 18.44 | HIGL |
| ATOM | 1461 | C   | ASN | 181 | 25.763 | 62.034 | 113.742 | 1.00 | 15.63 | HIGL |
| ATOM | 1462 | O   | ASN | 181 | 26.433 | 62.200 | 112.731 | 1.00 | 15.55 | HIGL |
| ATOM | 1463 | N   | GLY | 182 | 24.508 | 62.455 | 113.847 | 1.00 | 15.79 | HIGL |
| ATOM | 1464 | CA  | GLY | 182 | 23.853 | 63.129 | 112.744 | 1.00 | 15.12 | HIGL |
| ATOM | 1465 | C   | GLY | 182 | 24.575 | 64.373 | 112.287 | 1.00 | 15.79 | HIGL |
| ATOM | 1466 | O   | GLY | 182 | 24.331 | 64.857 | 111.184 | 1.00 | 16.16 | HIGL |
| ATOM | 1467 | N   | TRP | 183 | 25.459 | 64.902 | 113.130 | 1.00 | 16.94 | HIGL |
| ATOM | 1468 | CA  | TRP | 183 | 26.227 | 66.100 | 112.784 | 1.00 | 16.80 | HIGL |
| ATOM | 1469 | CB  | TRP | 183 | 26.854 | 66.746 | 114.034 | 1.00 | 16.19 | HIGL |
| ATOM | 1470 | CG  | TRP | 183 | 27.735 | 65.829 | 114.837 | 1.00 | 14.99 | HIGL |
| ATOM | 1471 | CD2 | TRP | 183 | 29.108 | 65.506 | 114.577 | 1.00 | 14.85 | HIGL |
| ATOM | 1472 | CE2 | TRP | 183 | 29.505 | 64.558 | 115.547 | 1.00 | 14.72 | HIGL |
| ATOM | 1473 | CE3 | TRP | 183 | 30.041 | 65.922 | 113.616 | 1.00 | 15.26 | HIGL |
| ATOM | 1474 | CD1 | TRP | 183 | 27.369 | 65.091 | 115.919 | 1.00 | 15.04 | HIGL |
| ATOM | 1475 | NE1 | TRP | 183 | 28.424 | 64.324 | 116.353 | 1.00 | 14.56 | HIGL |
| ATOM | 1476 | CZ2 | TRP | 183 | 30.798 | 64.015 | 115.586 | 1.00 | 13.96 | HIGL |
| ATOM | 1477 | CZ3 | TRP | 183 | 31.332 | 65.379 | 113.654 | 1.00 | 14.45 | HIGL |
| ATOM | 1478 | CH2 | TRP | 183 | 31.693 | 64.436 | 114.634 | 1.00 | 13.99 | HIGL |
| ATOM | 1479 | C   | TRP | 183 | 27.333 | 65.755 | 111.797 | 1.00 | 17.18 | HIGL |
| ATOM | 1480 | O   | TRP | 183 | 27.780 | 66.606 | 111.040 | 1.00 | 18.90 | HIGL |
| ATOM | 1481 | N   | ASN | 184 | 27.780 | 64.508 | 111.807 | 1.00 | 17.37 | HIGL |
| ATOM | 1482 | CA  | ASN | 184 | 28.838 | 64.087 | 110.901 | 1.00 | 18.52 | HIGL |
| ATOM | 1483 | CB  | ASN | 184 | 29.623 | 62.936 | 111.514 | 1.00 | 18.43 | HIGL |
| ATOM | 1484 | CG  | ASN | 184 | 30.892 | 62.651 | 110.760 | 1.00 | 18.15 | HIGL |
| ATOM | 1485 | OD1 | ASN | 184 | 30.904 | 62.652 | 109.528 | 1.00 | 17.65 | HIGL |
| ATOM | 1486 | ND2 | ASN | 184 | 31.972 | 62.403 | 111.490 | 1.00 | 16.66 | HIGL |
| ATOM | 1487 | C   | ASN | 184 | 28.265 | 63.647 | 109.551 | 1.00 | 19.20 | HIGL |
| ATOM | 1488 | O   | ASN | 184 | 27.800 | 62.515 | 109.406 | 1.00 | 19.59 | HIGL |
| ATOM | 1489 | N   | TRP | 185 | 28.318 | 64.536 | 108.563 | 1.00 | 18.87 | HIGL |
| ATOM | 1490 | CA  | TRP | 185 | 27.780 | 64.239 | 107.246 | 1.00 | 18.50 | HIGL |
| ATOM | 1491 | CB  | TRP | 185 | 27.752 | 65.517 | 106.404 | 1.00 | 19.66 | HIGL |
| ATOM | 1492 | CG  | TRP | 185 | 27.658 | 65.269 | 104.923 | 1.00 | 20.74 | HIGL |
| ATOM | 1493 | CD2 | TRP | 185 | 26.584 | 64.623 | 104.224 | 1.00 | 21.65 | HIGL |
| ATOM | 1494 | CE2 | TRP | 185 | 26.952 | 64.564 | 102.857 | 1.00 | 21.97 | HIGL |

# Fig. 2 cont.

| ATOM | 1495 | CE3 | TRP | 185 | 25.349 | 64.085 | 104.618 | 1.00 | 21.22 | HIGL |
|------|------|-----|-----|-----|--------|--------|---------|------|-------|------|
| ATOM | 1496 | CD1 | TRP | 185 | 28.601 | 65.570 | 103.982 | 1.00 | 20.45 | HIGL |
| ATOM | 1497 | NE1 | TRP | 185 | 28.184 | 65.151 | 102.740 | 1.00 | 21.70 | HIGL |
| ATOM | 1498 | CZ2 | TRP | 185 | 26.127 | 63.985 | 101.880 | 1.00 | 21.82 | HIGL |
| ATOM | 1499 | CZ3 | TRP | 185 | 24.526 | 63.509 | 103.645 | 1.00 | 21.31 | HIGL |
| ATOM | 1500 | CH2 | TRP | 185 | 24.921 | 63.465 | 102.292 | 1.00 | 21.28 | HIGL |
| ATOM | 1501 | C | TRP | 185 | 28.510 | 63.126 | 106.489 | 1.00 | 18.87 | HIGL |
| ATOM | 1502 | O | TRP | 185 | 27.873 | 62.328 | 105.796 | 1.00 | 18.21 | HIGL |
| ATOM | 1503 | N | ASP | 186 | 29.835 | 63.074 | 106.606 | 1.00 | 18.26 | HIGL |
| ATOM | 1504 | CA | ASP | 186 | 30.595 | 62.042 | 105.918 | 1.00 | 18.41 | HIGL |
| ATOM | 1505 | CB | ASP | 186 | 32.094 | 62.185 | 106.181 | 1.00 | 19.07 | HIGL |
| ATOM | 1506 | CG | ASP | 186 | 32.662 | 63.492 | 105.644 | 1.00 | 19.86 | HIGL |
| ATOM | 1507 | OD1 | ASP | 186 | 32.235 | 63.922 | 104.546 | 1.00 | 18.31 | HIGL |
| ATOM | 1508 | OD2 | ASP | 186 | 33.539 | 64.082 | 106.321 | 1.00 | 20.67 | HIGL |
| ATOM | 1509 | C | ASP | 186 | 30.127 | 60.669 | 106.375 | 1.00 | 18.79 | HIGL |
| ATOM | 1510 | O | ASP | 186 | 30.057 | 59.738 | 105.569 | 1.00 | 19.44 | HIGL |
| ATOM | 1511 | N | THR | 187 | 29.804 | 60.541 | 107.662 | 1.00 | 18.54 | HIGL |
| ATOM | 1512 | CA | THR | 187 | 29.326 | 59.267 | 108.185 | 1.00 | 18.36 | HIGL |
| ATOM | 1513 | CB | THR | 187 | 29.144 | 59.303 | 109.717 | 1.00 | 18.81 | HIGL |
| ATOM | 1514 | OG1 | THR | 187 | 30.334 | 59.779 | 110.359 | 1.00 | 17.18 | HIGL |
| ATOM | 1515 | CG2 | THR | 187 | 28.841 | 57.898 | 110.229 | 1.00 | 17.29 | HIGL |
| ATOM | 1516 | C | THR | 187 | 27.955 | 58.970 | 107.554 | 1.00 | 18.81 | HIGL |
| ATOM | 1517 | O | THR | 187 | 27.749 | 57.924 | 106.953 | 1.00 | 18.82 | HIGL |
| ATOM | 1518 | N | GLN | 188 | 27.028 | 59.912 | 107.690 | 1.00 | 18.92 | HIGL |
| ATOM | 1519 | CA | GLN | 188 | 25.678 | 59.756 | 107.123 | 1.00 | 18.70 | HIGL |
| ATOM | 1520 | CB | GLN | 188 | 24.868 | 61.025 | 107.278 | 1.00 | 18.92 | HIGL |
| ATOM | 1521 | CG | GLN | 188 | 24.691 | 61.548 | 108.719 | 1.00 | 20.75 | HIGL |
| ATOM | 1522 | CD | GLN | 188 | 24.217 | 60.494 | 109.715 | 1.00 | 21.45 | HIGL |
| ATOM | 1523 | OE1 | GLN | 188 | 23.340 | 59.658 | 109.425 | 1.00 | 21.55 | HIGL |
| ATOM | 1524 | NE2 | GLN | 188 | 24.775 | 60.558 | 110.916 | 1.00 | 20.88 | HIGL |
| ATOM | 1525 | C | GLN | 188 | 25.693 | 59.419 | 105.628 | 1.00 | 18.27 | HIGL |
| ATOM | 1526 | O | GLN | 188 | 24.854 | 58.643 | 105.144 | 1.00 | 19.06 | HIGL |
| ATOM | 1527 | N | ASN | 189 | 26.652 | 60.019 | 104.912 | 1.00 | 18.01 | HIGL |
| ATOM | 1528 | CA | ASN | 189 | 26.837 | 59.855 | 103.466 | 1.00 | 17.83 | HIGL |
| ATOM | 1529 | CB | ASN | 189 | 27.713 | 61.007 | 102.897 | 1.00 | 18.12 | HIGL |
| ATOM | 1530 | CG | ASN | 189 | 27.816 | 60.975 | 101.367 | 1.00 | 18.97 | HIGL |
| ATOM | 1531 | OD1 | ASN | 189 | 27.022 | 60.302 | 100.708 | 1.00 | 18.06 | HIGL |
| ATOM | 1532 | ND2 | ASN | 189 | 28.776 | 61.718 | 100.800 | 1.00 | 19.12 | HIGL |
| ATOM | 1533 | C | ASN | 189 | 27.460 | 58.493 | 103.165 | 1.00 | 17.73 | HIGL |
| ATOM | 1534 | O | ASN | 189 | 26.935 | 57.760 | 102.331 | 1.00 | 17.69 | HIGL |
| ATOM | 1535 | N | TRP | 190 | 28.583 | 58.180 | 103.812 | 1.00 | 17.17 | HIGL |
| ATOM | 1536 | CA | TRP | 190 | 29.272 | 56.895 | 103.656 | 1.00 | 16.53 | HIGL |
| ATOM | 1537 | CB | TRP | 190 | 30.409 | 56.855 | 104.679 | 1.00 | 16.92 | HIGL |
| ATOM | 1538 | CG | TRP | 190 | 30.943 | 55.516 | 105.033 | 1.00 | 17.78 | HIGL |
| ATOM | 1539 | CD2 | TRP | 190 | 30.714 | 54.794 | 106.253 | 1.00 | 17.06 | HIGL |
| ATOM | 1540 | CE2 | TRP | 190 | 31.490 | 53.620 | 106.192 | 1.00 | 18.29 | HIGL |
| ATOM | 1541 | CE3 | TRP | 190 | 29.931 | 55.028 | 107.392 | 1.00 | 17.68 | HIGL |
| ATOM | 1542 | CD1 | TRP | 190 | 31.811 | 54.770 | 104.303 | 1.00 | 18.04 | HIGL |
| ATOM | 1543 | NE1 | TRP | 190 | 32.150 | 53.630 | 104.991 | 1.00 | 18.09 | HIGL |
| ATOM | 1544 | CZ2 | TRP | 190 | 31.511 | 52.675 | 107.230 | 1.00 | 18.43 | HIGL |
| ATOM | 1545 | CZ3 | TRP | 190 | 29.951 | 54.083 | 108.431 | 1.00 | 18.02 | HIGL |
| ATOM | 1546 | CH2 | TRP | 190 | 30.738 | 52.925 | 108.336 | 1.00 | 17.37 | HIGL |
| ATOM | 1547 | C | TRP | 190 | 28.307 | 55.715 | 103.874 | 1.00 | 15.60 | HIGL |
| ATOM | 1548 | O | TRP | 190 | 28.193 | 54.800 | 103.053 | 1.00 | 16.16 | HIGL |
| ATOM | 1549 | N | TRP | 191 | 27.609 | 55.744 | 104.997 | 1.00 | 14.48 | HIGL |
| ATOM | 1550 | CA | TRP | 191 | 26.674 | 54.686 | 105.327 | 1.00 | 14.21 | HIGL |
| ATOM | 1551 | CB | TRP | 191 | 26.028 | 54.956 | 106.681 | 1.00 | 12.41 | HIGL |
| ATOM | 1552 | CG | TRP | 191 | 25.437 | 53.729 | 107.273 | 1.00 | 11.51 | HIGL |
| ATOM | 1553 | CD2 | TRP | 191 | 24.101 | 53.250 | 107.097 | 1.00 | 10.28 | HIGL |
| ATOM | 1554 | CE2 | TRP | 191 | 23.990 | 52.044 | 107.827 | 1.00 | 10.64 | HIGL |
| ATOM | 1555 | CE3 | TRP | 191 | 22.986 | 53.720 | 106.393 | 1.00 | 7.88 | HIGL |
| ATOM | 1556 | CD1 | TRP | 191 | 26.068 | 52.820 | 108.074 | 1.00 | 12.10 | HIGL |
| ATOM | 1557 | NE1 | TRP | 191 | 25.208 | 51.805 | 108.413 | 1.00 | 10.86 | HIGL |
| ATOM | 1558 | CZ2 | TRP | 191 | 22.808 | 51.304 | 107.876 | 1.00 | 9.13 | HIGL |
| ATOM | 1559 | CZ3 | TRP | 191 | 21.818 | 52.988 | 106.440 | 1.00 | 8.78 | HIGL |

# Fig. 2 cont.

| ATOM | 1560 | CH2 | TRP | 191 | 21.735 | 51.790 | 107.178 | 1.00 | 9.52 | HIGL |
|------|------|-----|-----|-----|--------|--------|---------|------|------|------|
| ATOM | 1561 | C | TRP | 191 | 25.566 | 54.471 | 104.292 | 1.00 | 14.99 | HIGL |
| ATOM | 1562 | O | TRP | 191 | 25.485 | 53.409 | 103.664 | 1.00 | 14.62 | HIGL |
| ATOM | 1563 | N | TYR | 192 | 24.703 | 55.468 | 104.121 | 1.00 | 15.56 | HIGL |
| ATOM | 1564 | CA | TYR | 192 | 23.595 | 55.341 | 103.178 | 1.00 | 16.00 | HIGL |
| ATOM | 1565 | CB | TYR | 192 | 22.739 | 56.615 | 103.195 | 1.00 | 15.03 | HIGL |
| ATOM | 1566 | CG | TYR | 192 | 21.859 | 56.737 | 104.428 | 1.00 | 14.42 | HIGL |
| ATOM | 1567 | CD1 | TYR | 192 | 20.759 | 55.886 | 104.617 | 1.00 | 14.00 | HIGL |
| ATOM | 1568 | CE1 | TYR | 192 | 19.954 | 55.987 | 105.746 | 1.00 | 13.21 | HIGL |
| ATOM | 1569 | CD2 | TYR | 192 | 22.128 | 57.691 | 105.408 | 1.00 | 13.33 | HIGL |
| ATOM | 1570 | CE2 | TYR | 192 | 21.332 | 57.804 | 106.544 | 1.00 | 13.35 | HIGL |
| ATOM | 1571 | CZ | TYR | 192 | 20.244 | 56.950 | 106.709 | 1.00 | 13.89 | HIGL |
| ATOM | 1572 | OH | TYR | 192 | 19.442 | 57.073 | 107.826 | 1.00 | 12.40 | HIGL |
| ATOM | 1573 | C | TYR | 192 | 24.052 | 55.015 | 101.760 | 1.00 | 17.04 | HIGL |
| ATOM | 1574 | O | TYR | 192 | 23.433 | 54.199 | 101.071 | 1.00 | 17.52 | HIGL |
| ATOM | 1575 | N | THR | 193 | 25.137 | 55.643 | 101.325 | 1.00 | 17.90 | HIGL |
| ATOM | 1576 | CA | THR | 193 | 25.654 | 55.388 | 99.993 | 1.00 | 18.57 | HIGL |
| ATOM | 1577 | CB | THR | 193 | 26.949 | 56.186 | 99.738 | 1.00 | 19.70 | HIGL |
| ATOM | 1578 | OG1 | THR | 193 | 26.634 | 57.582 | 99.645 | 1.00 | 20.25 | HIGL |
| ATOM | 1579 | CG2 | THR | 193 | 27.629 | 55.716 | 98.441 | 1.00 | 17.66 | HIGL |
| ATOM | 1580 | C | THR | 193 | 25.950 | 53.897 | 99.842 | 1.00 | 18.55 | HIGL |
| ATOM | 1581 | O | THR | 193 | 25.442 | 53.230 | 98.937 | 1.00 | 18.73 | HIGL |
| ATOM | 1582 | N | ASN | 194 | 26.772 | 53.377 | 100.742 | 1.00 | 17.82 | HIGL |
| ATOM | 1583 | CA | ASN | 194 | 27.127 | 51.972 | 100.693 | 1.00 | 18.02 | HIGL |
| ATOM | 1584 | CB | ASN | 194 | 28.166 | 51.663 | 101.762 | 1.00 | 17.18 | HIGL |
| ATOM | 1585 | CG | ASN | 194 | 29.546 | 52.148 | 101.381 | 1.00 | 16.79 | HIGL |
| ATOM | 1586 | OD1 | ASN | 194 | 30.135 | 51.668 | 100.411 | 1.00 | 17.28 | HIGL |
| ATOM | 1587 | ND2 | ASN | 194 | 30.073 | 53.102 | 102.137 | 1.00 | 16.49 | HIGL |
| ATOM | 1588 | C | ASN | 194 | 25.934 | 51.031 | 100.830 | 1.00 | 18.35 | HIGL |
| ATOM | 1589 | O | ASN | 194 | 25.860 | 50.029 | 100.123 | 1.00 | 20.21 | HIGL |
| ATOM | 1590 | N | VAL | 195 | 25.003 | 51.345 | 101.724 | 1.00 | 17.31 | HIGL |
| ATOM | 1591 | CA | VAL | 195 | 23.838 | 50.495 | 101.908 | 1.00 | 17.12 | HIGL |
| ATOM | 1592 | CB | VAL | 195 | 23.052 | 50.887 | 103.185 | 1.00 | 17.17 | HIGL |
| ATOM | 1593 | CG1 | VAL | 195 | 21.789 | 50.062 | 103.290 | 1.00 | 16.39 | HIGL |
| ATOM | 1594 | CG2 | VAL | 195 | 23.906 | 50.675 | 104.411 | 1.00 | 16.35 | HIGL |
| ATOM | 1595 | C | VAL | 195 | 22.882 | 50.550 | 100.711 | 1.00 | 17.84 | HIGL |
| ATOM | 1596 | O | VAL | 195 | 22.414 | 49.514 | 100.223 | 1.00 | 17.57 | HIGL |
| ATOM | 1597 | N | LEU | 196 | 22.591 | 51.755 | 100.234 | 1.00 | 17.80 | HIGL |
| ATOM | 1598 | CA | LEU | 196 | 21.672 | 51.906 | 99.114 | 1.00 | 18.71 | HIGL |
| ATOM | 1599 | CB | LEU | 196 | 21.164 | 53.346 | 99.049 | 1.00 | 19.05 | HIGL |
| ATOM | 1600 | CG | LEU | 196 | 20.389 | 53.814 | 100.284 | 1.00 | 19.84 | HIGL |
| ATOM | 1601 | CD1 | LEU | 196 | 19.935 | 55.255 | 100.071 | 1.00 | 19.18 | HIGL |
| ATOM | 1602 | CD2 | LEU | 196 | 19.188 | 52.901 | 100.532 | 1.00 | 18.91 | HIGL |
| ATOM | 1603 | C | LEU | 196 | 22.219 | 51.490 | 97.745 | 1.00 | 18.86 | HIGL |
| ATOM | 1604 | O | LEU | 196 | 21.446 | 51.326 | 96.798 | 1.00 | 18.34 | HIGL |
| ATOM | 1605 | N | SER | 197 | 23.537 | 51.316 | 97.631 | 1.00 | 18.55 | HIGL |
| ATOM | 1606 | CA | SER | 197 | 24.126 | 50.913 | 96.355 | 1.00 | 18.26 | HIGL |
| ATOM | 1607 | CB | SER | 197 | 25.561 | 51.426 | 96.232 | 1.00 | 17.73 | HIGL |
| ATOM | 1608 | OG | SER | 197 | 26.436 | 50.722 | 97.091 | 1.00 | 18.32 | HIGL |
| ATOM | 1609 | C | SER | 197 | 24.113 | 49.397 | 96.184 | 1.00 | 18.38 | HIGL |
| ATOM | 1610 | O | SER | 197 | 24.322 | 48.884 | 95.088 | 1.00 | 18.24 | HIGL |
| ATOM | 1611 | N | GLN | 198 | 23.859 | 48.677 | 97.269 | 1.00 | 18.80 | HIGL |
| ATOM | 1612 | CA | GLN | 198 | 23.822 | 47.223 | 97.212 | 1.00 | 18.22 | HIGL |
| ATOM | 1613 | CB | GLN | 198 | 23.686 | 46.653 | 98.620 | 1.00 | 19.28 | HIGL |
| ATOM | 1614 | CG | GLN | 198 | 24.836 | 46.994 | 99.518 | 1.00 | 19.81 | HIGL |
| ATOM | 1615 | CD | GLN | 198 | 26.161 | 46.734 | 98.847 | 1.00 | 21.32 | HIGL |
| ATOM | 1616 | OE1 | GLN | 198 | 26.353 | 45.693 | 98.210 | 1.00 | 21.68 | HIGL |
| ATOM | 1617 | NE2 | GLN | 198 | 27.091 | 47.679 | 98.984 | 1.00 | 21.99 | HIGL |
| ATOM | 1618 | C | GLN | 198 | 22.682 | 46.707 | 96.340 | 1.00 | 17.65 | HIGL |
| ATOM | 1619 | O | GLN | 198 | 22.877 | 45.821 | 95.514 | 1.00 | 17.50 | HIGL |
| ATOM | 1620 | N | GLY | 199 | 21.486 | 47.253 | 96.536 | 1.00 | 17.03 | HIGL |
| ATOM | 1621 | CA | GLY | 199 | 20.347 | 46.821 | 95.745 | 1.00 | 15.62 | HIGL |
| ATOM | 1622 | C | GLY | 199 | 19.181 | 46.278 | 96.560 | 1.00 | 15.72 | HIGL |
| ATOM | 1623 | O | GLY | 199 | 18.045 | 46.710 | 96.364 | 1.00 | 15.60 | HIGL |
| ATOM | 1624 | N | PRO | 200 | 19.422 | 45.336 | 97.488 | 1.00 | 15.34 | HIGL |

# Fig. 2 cont.

| ATOM | 1625 | CD  | PRO | 200 | 20.704 | 44.672 | 97.783  | 1.00 | 14.88 | HIGL |
|------|------|-----|-----|-----|--------|--------|---------|------|-------|------|
| ATOM | 1626 | CA  | PRO | 200 | 18.350 | 44.764 | 98.306  | 1.00 | 14.92 | HIGL |
| ATOM | 1627 | CB  | PRO | 200 | 19.104 | 43.814 | 99.225  | 1.00 | 16.05 | HIGL |
| ATOM | 1628 | CG  | PRO | 200 | 20.245 | 43.367 | 98.366  | 1.00 | 14.92 | HIGL |
| ATOM | 1629 | C   | PRO | 200 | 17.518 | 45.794 | 99.076  | 1.00 | 15.90 | HIGL |
| ATOM | 1630 | O   | PRO | 200 | 16.288 | 45.699 | 99.112  | 1.00 | 14.94 | HIGL |
| ATOM | 1631 | N   | PHE | 201 | 18.178 | 46.771 | 99.698  | 1.00 | 16.66 | HIGL |
| ATOM | 1632 | CA  | PHE | 201 | 17.457 | 47.806 | 100.439 | 1.00 | 17.91 | HIGL |
| ATOM | 1633 | CB  | PHE | 201 | 18.296 | 48.317 | 101.607 | 1.00 | 17.39 | HIGL |
| ATOM | 1634 | CG  | PHE | 201 | 17.523 | 49.154 | 102.585 | 1.00 | 16.03 | HIGL |
| ATOM | 1635 | CD1 | PHE | 201 | 16.320 | 48.696 | 103.108 | 1.00 | 15.39 | HIGL |
| ATOM | 1636 | CD2 | PHE | 201 | 18.019 | 50.376 | 103.019 | 1.00 | 16.33 | HIGL |
| ATOM | 1637 | CE1 | PHE | 201 | 15.627 | 49.436 | 104.049 | 1.00 | 16.04 | HIGL |
| ATOM | 1638 | CE2 | PHE | 201 | 17.331 | 51.130 | 103.967 | 1.00 | 16.47 | HIGL |
| ATOM | 1639 | CZ  | PHE | 201 | 16.133 | 50.658 | 104.484 | 1.00 | 16.02 | HIGL |
| ATOM | 1640 | C   | PHE | 201 | 17.160 | 48.947 | 99.481  | 1.00 | 19.32 | HIGL |
| ATOM | 1641 | O   | PHE | 201 | 18.052 | 49.707 | 99.113  | 1.00 | 19.83 | HIGL |
| ATOM | 1642 | N   | GLU | 202 | 15.899 | 49.066 | 99.088  | 1.00 | 20.88 | HIGL |
| ATOM | 1643 | CA  | GLU | 202 | 15.492 | 50.079 | 98.130  | 1.00 | 22.59 | HIGL |
| ATOM | 1644 | CB  | GLU | 202 | 14.381 | 49.527 | 97.248  | 1.00 | 25.23 | HIGL |
| ATOM | 1645 | CG  | GLU | 202 | 14.646 | 48.127 | 96.733  | 1.00 | 29.70 | HIGL |
| ATOM | 1646 | CD  | GLU | 202 | 13.649 | 47.709 | 95.670  | 1.00 | 31.92 | HIGL |
| ATOM | 1647 | OE1 | GLU | 202 | 13.642 | 48.342 | 94.588  | 1.00 | 33.85 | HIGL |
| ATOM | 1648 | OE2 | GLU | 202 | 12.876 | 46.758 | 95.916  | 1.00 | 32.65 | HIGL |
| ATOM | 1649 | C   | GLU | 202 | 15.033 | 51.394 | 98.724  | 1.00 | 22.89 | HIGL |
| ATOM | 1650 | O   | GLU | 202 | 14.660 | 51.473 | 99.892  | 1.00 | 23.53 | HIGL |
| ATOM | 1651 | N   | MET | 203 | 15.046 | 52.426 | 97.891  | 1.00 | 23.12 | HIGL |
| ATOM | 1652 | CA  | MET | 203 | 14.624 | 53.748 | 98.309  | 1.00 | 23.40 | HIGL |
| ATOM | 1653 | CB  | MET | 203 | 14.768 | 54.734 | 97.153  | 1.00 | 24.47 | HIGL |
| ATOM | 1654 | CG  | MET | 203 | 16.202 | 55.007 | 96.767  | 1.00 | 27.52 | HIGL |
| ATOM | 1655 | SD  | MET | 203 | 17.161 | 55.583 | 98.175  | 1.00 | 30.04 | HIGL |
| ATOM | 1656 | CE  | MET | 203 | 16.411 | 57.199 | 98.411  | 1.00 | 29.30 | HIGL |
| ATOM | 1657 | C   | MET | 203 | 13.185 | 53.748 | 98.808  | 1.00 | 22.78 | HIGL |
| ATOM | 1658 | O   | MET | 203 | 12.835 | 54.522 | 99.696  | 1.00 | 22.95 | HIGL |
| ATOM | 1659 | N   | SER | 204 | 12.352 | 52.878 | 98.251  | 1.00 | 21.87 | HIGL |
| ATOM | 1660 | CA  | SER | 204 | 10.956 | 52.823 | 98.668  | 1.00 | 21.55 | HIGL |
| ATOM | 1661 | CB  | SER | 204 | 10.077 | 52.307 | 97.521  | 1.00 | 21.02 | HIGL |
| ATOM | 1662 | OG  | SER | 204 | 10.458 | 51.006 | 97.107  | 1.00 | 20.98 | HIGL |
| ATOM | 1663 | C   | SER | 204 | 10.741 | 51.961 | 99.913  | 1.00 | 21.58 | HIGL |
| ATOM | 1664 | O   | SER | 204 | 9.610  | 51.822 | 100.379 | 1.00 | 21.09 | HIGL |
| ATOM | 1665 | N   | ASP | 205 | 11.821 | 51.388 | 100.448 | 1.00 | 20.89 | HIGL |
| ATOM | 1666 | CA  | ASP | 205 | 11.723 | 50.545 | 101.640 | 1.00 | 20.32 | HIGL |
| ATOM | 1667 | CB  | ASP | 205 | 12.882 | 49.539 | 101.716 | 1.00 | 20.48 | HIGL |
| ATOM | 1668 | CG  | ASP | 205 | 12.750 | 48.411 | 100.710 | 1.00 | 19.95 | HIGL |
| ATOM | 1669 | OD1 | ASP | 205 | 11.607 | 47.992 | 100.424 | 1.00 | 20.12 | HIGL |
| ATOM | 1670 | OD2 | ASP | 205 | 13.792 | 47.933 | 100.220 | 1.00 | 19.93 | HIGL |
| ATOM | 1671 | C   | ASP | 205 | 11.681 | 51.325 | 102.944 | 1.00 | 19.69 | HIGL |
| ATOM | 1672 | O   | ASP | 205 | 11.284 | 50.780 | 103.971 | 1.00 | 19.83 | HIGL |
| ATOM | 1673 | N   | PHE | 206 | 12.109 | 52.584 | 102.927 | 1.00 | 19.32 | HIGL |
| ATOM | 1674 | CA  | PHE | 206 | 12.062 | 53.377 | 104.149 | 1.00 | 19.43 | HIGL |
| ATOM | 1675 | CB  | PHE | 206 | 13.413 | 53.376 | 104.877 | 1.00 | 19.75 | HIGL |
| ATOM | 1676 | CG  | PHE | 206 | 14.492 | 54.155 | 104.194 | 1.00 | 20.11 | HIGL |
| ATOM | 1677 | CD1 | PHE | 206 | 14.975 | 53.768 | 102.951 | 1.00 | 20.98 | HIGL |
| ATOM | 1678 | CD2 | PHE | 206 | 15.090 | 55.233 | 104.839 | 1.00 | 19.93 | HIGL |
| ATOM | 1679 | CE1 | PHE | 206 | 16.048 | 54.442 | 102.364 | 1.00 | 20.58 | HIGL |
| ATOM | 1680 | CE2 | PHE | 206 | 16.154 | 55.908 | 104.264 | 1.00 | 19.23 | HIGL |
| ATOM | 1681 | CZ  | PHE | 206 | 16.636 | 55.509 | 103.025 | 1.00 | 19.95 | HIGL |
| ATOM | 1682 | C   | PHE | 206 | 11.588 | 54.791 | 103.900 | 1.00 | 19.04 | HIGL |
| ATOM | 1683 | O   | PHE | 206 | 11.597 | 55.267 | 102.773 | 1.00 | 19.32 | HIGL |
| ATOM | 1684 | N   | ASP | 207 | 11.173 | 55.462 | 104.965 | 1.00 | 19.22 | HIGL |
| ATOM | 1685 | CA  | ASP | 207 | 10.636 | 56.810 | 104.841 | 1.00 | 19.23 | HIGL |
| ATOM | 1686 | CB  | ASP | 207 | 9.175  | 56.802 | 105.286 | 1.00 | 19.16 | HIGL |
| ATOM | 1687 | CG  | ASP | 207 | 8.407  | 55.625 | 104.718 | 1.00 | 19.38 | HIGL |
| ATOM | 1688 | OD1 | ASP | 207 | 8.277  | 55.543 | 103.480 | 1.00 | 20.06 | HIGL |
| ATOM | 1689 | OD2 | ASP | 207 | 7.942  | 54.778 | 105.507 | 1.00 | 18.36 | HIGL |

# Fig. 2 cont.

| ATOM | 1690 | C | ASP | 207 | 11.381 | 57.871 | 105.629 | 1.00 | 18.86 | HIGL |
|------|------|-----|-----|-----|--------|--------|---------|------|-------|------|
| ATOM | 1691 | O | ASP | 207 | 11.381 | 59.045 | 105.260 | 1.00 | 19.26 | HIGL |
| ATOM | 1692 | N | MET | 208 | 12.015 | 57.466 | 106.716 | 1.00 | 18.21 | HIGL |
| ATOM | 1693 | CA | MET | 208 | 12.714 | 58.433 | 107.540 | 1.00 | 18.11 | HIGL |
| ATOM | 1694 | CB | MET | 208 | 12.006 | 58.596 | 108.894 | 1.00 | 18.41 | HIGL |
| ATOM | 1695 | CG | MET | 208 | 10.534 | 58.987 | 108.820 | 1.00 | 20.52 | HIGL |
| ATOM | 1696 | SD | MET | 208 | 9.808 | 59.310 | 110.452 | 1.00 | 22.01 | HIGL |
| ATOM | 1697 | CE | MET | 208 | 10.379 | 60.977 | 110.731 | 1.00 | 20.87 | HIGL |
| ATOM | 1698 | C | MET | 208 | 14.161 | 58.083 | 107.804 | 1.00 | 17.69 | HIGL |
| ATOM | 1699 | O | MET | 208 | 14.579 | 56.928 | 107.707 | 1.00 | 17.61 | HIGL |
| ATOM | 1700 | N | MET | 209 | 14.918 | 59.119 | 108.129 | 1.00 | 16.92 | HIGL |
| ATOM | 1701 | CA | MET | 209 | 16.308 | 58.994 | 108.488 | 1.00 | 16.07 | HIGL |
| ATOM | 1702 | CB | MET | 209 | 17.213 | 59.645 | 107.443 | 1.00 | 16.00 | HIGL |
| ATOM | 1703 | CG | MET | 209 | 17.373 | 58.828 | 106.170 | 1.00 | 16.81 | HIGL |
| ATOM | 1704 | SD | MET | 209 | 18.554 | 59.575 | 105.009 | 1.00 | 19.85 | HIGL |
| ATOM | 1705 | CE | MET | 209 | 18.496 | 58.407 | 103.621 | 1.00 | 17.63 | HIGL |
| ATOM | 1706 | C | MET | 209 | 16.374 | 59.747 | 109.809 | 1.00 | 16.16 | HIGL |
| ATOM | 1707 | O | MET | 209 | 16.174 | 60.969 | 109.850 | 1.00 | 15.45 | HIGL |
| ATOM | 1708 | N | GLY | 210 | 16.600 | 59.001 | 110.891 | 1.00 | 15.65 | HIGL |
| ATOM | 1709 | CA | GLY | 210 | 16.695 | 59.603 | 112.210 | 1.00 | 14.42 | HIGL |
| ATOM | 1710 | C | GLY | 210 | 18.150 | 59.686 | 112.629 | 1.00 | 14.08 | HIGL |
| ATOM | 1711 | O | GLY | 210 | 18.961 | 58.883 | 112.175 | 1.00 | 13.68 | HIGL |
| ATOM | 1712 | N | VAL | 211 | 18.490 | 60.651 | 113.484 | 1.00 | 13.61 | HIGL |
| ATOM | 1713 | CA | VAL | 211 | 19.869 | 60.802 | 113.936 | 1.00 | 13.15 | HIGL |
| ATOM | 1714 | CB | VAL | 211 | 20.627 | 61.892 | 113.141 | 1.00 | 12.33 | HIGL |
| ATOM | 1715 | CG1 | VAL | 211 | 20.537 | 61.611 | 111.663 | 1.00 | 13.18 | HIGL |
| ATOM | 1716 | CG2 | VAL | 211 | 20.067 | 63.271 | 113.465 | 1.00 | 11.20 | HIGL |
| ATOM | 1717 | C | VAL | 211 | 19.984 | 61.175 | 115.400 | 1.00 | 13.77 | HIGL |
| ATOM | 1718 | O | VAL | 211 | 19.118 | 61.837 | 115.958 | 1.00 | 13.69 | HIGL |
| ATOM | 1719 | N | SER | 212 | 21.069 | 60.741 | 116.022 | 1.00 | 15.09 | HIGL |
| ATOM | 1720 | CA | SER | 212 | 21.313 | 61.079 | 117.411 | 1.00 | 15.93 | HIGL |
| ATOM | 1721 | CB | SER | 212 | 22.016 | 59.929 | 118.130 | 1.00 | 16.46 | HIGL |
| ATOM | 1722 | OG | SER | 212 | 21.185 | 58.781 | 118.176 | 1.00 | 17.21 | HIGL |
| ATOM | 1723 | C | SER | 212 | 22.208 | 62.315 | 117.376 | 1.00 | 16.32 | HIGL |
| ATOM | 1724 | O | SER | 212 | 23.149 | 62.395 | 116.582 | 1.00 | 16.25 | HIGL |
| ATOM | 1725 | N | PHE | 213 | 21.890 | 63.289 | 118.214 | 1.00 | 15.47 | HIGL |
| ATOM | 1726 | CA | PHE | 213 | 22.666 | 64.512 | 118.267 | 1.00 | 15.45 | HIGL |
| ATOM | 1727 | CB | PHE | 213 | 21.923 | 65.634 | 117.528 | 1.00 | 15.73 | HIGL |
| ATOM | 1728 | CG | PHE | 213 | 22.673 | 66.936 | 117.484 | 1.00 | 16.40 | HIGL |
| ATOM | 1729 | CD1 | PHE | 213 | 23.883 | 67.036 | 116.799 | 1.00 | 16.45 | HIGL |
| ATOM | 1730 | CD2 | PHE | 213 | 22.183 | 68.057 | 118.146 | 1.00 | 16.56 | HIGL |
| ATOM | 1731 | CE1 | PHE | 213 | 24.596 | 68.231 | 116.777 | 1.00 | 15.36 | HIGL |
| ATOM | 1732 | CE2 | PHE | 213 | 22.889 | 69.257 | 118.130 | 1.00 | 16.74 | HIGL |
| ATOM | 1733 | CZ | PHE | 213 | 24.100 | 69.340 | 117.443 | 1.00 | 16.06 | HIGL |
| ATOM | 1734 | C | PHE | 213 | 22.849 | 64.850 | 119.738 | 1.00 | 14.96 | HIGL |
| ATOM | 1735 | O | PHE | 213 | 21.888 | 65.175 | 120.436 | 1.00 | 15.30 | HIGL |
| ATOM | 1736 | N | TYR | 214 | 24.085 | 64.742 | 120.208 | 1.00 | 14.20 | HIGL |
| ATOM | 1737 | CA | TYR | 214 | 24.420 | 65.016 | 121.600 | 1.00 | 13.58 | HIGL |
| ATOM | 1738 | CB | TYR | 214 | 24.875 | 63.736 | 122.298 | 1.00 | 12.69 | HIGL |
| ATOM | 1739 | CG | TYR | 214 | 23.775 | 62.742 | 122.558 | 1.00 | 11.90 | HIGL |
| ATOM | 1740 | CD1 | TYR | 214 | 22.902 | 62.906 | 123.631 | 1.00 | 11.71 | HIGL |
| ATOM | 1741 | CE1 | TYR | 214 | 21.885 | 61.989 | 123.874 | 1.00 | 11.65 | HIGL |
| ATOM | 1742 | CD2 | TYR | 214 | 23.602 | 61.635 | 121.731 | 1.00 | 10.99 | HIGL |
| ATOM | 1743 | CE2 | TYR | 214 | 22.591 | 60.717 | 121.962 | 1.00 | 11.61 | HIGL |
| ATOM | 1744 | CZ | TYR | 214 | 21.735 | 60.899 | 123.035 | 1.00 | 11.76 | HIGL |
| ATOM | 1745 | OH | TYR | 214 | 20.722 | 59.997 | 123.259 | 1.00 | 12.70 | HIGL |
| ATOM | 1746 | C | TYR | 214 | 25.541 | 66.035 | 121.660 | 1.00 | 14.26 | HIGL |
| ATOM | 1747 | O | TYR | 214 | 26.346 | 66.141 | 120.742 | 1.00 | 15.11 | HIGL |
| ATOM | 1748 | N | PRO | 215 | 25.619 | 66.794 | 122.755 | 1.00 | 14.63 | HIGL |
| ATOM | 1749 | CD | PRO | 215 | 24.581 | 67.036 | 123.775 | 1.00 | 14.17 | HIGL |
| ATOM | 1750 | CA | PRO | 215 | 26.682 | 67.790 | 122.847 | 1.00 | 14.95 | HIGL |
| ATOM | 1751 | CB | PRO | 215 | 25.990 | 68.930 | 123.572 | 1.00 | 14.94 | HIGL |
| ATOM | 1752 | CG | PRO | 215 | 25.175 | 68.176 | 124.596 | 1.00 | 14.41 | HIGL |
| ATOM | 1753 | C | PRO | 215 | 27.924 | 67.322 | 123.598 | 1.00 | 15.93 | HIGL |
| ATOM | 1754 | O | PRO | 215 | 28.999 | 67.898 | 123.437 | 1.00 | 16.94 | HIGL |

# Fig. 2 cont.

| ATOM | 1755 | N | PHE | 216 | 27.778 | 66.276 | 124.405 | 1.00 | 16.00 | HIGL |
|------|------|-----|-----|-----|--------|--------|---------|------|-------|------|
| ATOM | 1756 | CA | PHE | 216 | 28.878 | 65.791 | 125.231 | 1.00 | 16.24 | HIGL |
| ATOM | 1757 | CB | PHE | 216 | 28.350 | 65.520 | 126.644 | 1.00 | 16.24 | HIGL |
| ATOM | 1758 | CG | PHE | 216 | 27.018 | 64.792 | 126.677 | 1.00 | 16.08 | HIGL |
| ATOM | 1759 | CD1 | PHE | 216 | 26.861 | 63.555 | 126.055 | 1.00 | 15.04 | HIGL |
| ATOM | 1760 | CD2 | PHE | 216 | 25.924 | 65.347 | 127.343 | 1.00 | 15.16 | HIGL |
| ATOM | 1761 | CE1 | PHE | 216 | 25.638 | 62.889 | 126.095 | 1.00 | 15.26 | HIGL |
| ATOM | 1762 | CE2 | PHE | 216 | 24.703 | 64.686 | 127.386 | 1.00 | 14.85 | HIGL |
| ATOM | 1763 | CZ | PHE | 216 | 24.560 | 63.453 | 126.759 | 1.00 | 14.72 | HIGL |
| ATOM | 1764 | C | PHE | 216 | 29.709 | 64.595 | 124.763 | 1.00 | 16.64 | HIGL |
| ATOM | 1765 | O | PHE | 216 | 30.291 | 63.882 | 125.580 | 1.00 | 16.43 | HIGL |
| ATOM | 1766 | N | TYR | 217 | 29.789 | 64.377 | 123.459 | 1.00 | 17.14 | HIGL |
| ATOM | 1767 | CA | TYR | 217 | 30.582 | 63.260 | 122.947 | 1.00 | 17.62 | HIGL |
| ATOM | 1768 | CB | TYR | 217 | 29.675 | 62.193 | 122.323 | 1.00 | 16.27 | HIGL |
| ATOM | 1769 | CG | TYR | 217 | 28.847 | 61.399 | 123.315 | 1.00 | 16.34 | HIGL |
| ATOM | 1770 | CD1 | TYR | 217 | 29.440 | 60.785 | 124.421 | 1.00 | 16.29 | HIGL |
| ATOM | 1771 | CE1 | TYR | 217 | 28.687 | 60.024 | 125.312 | 1.00 | 15.97 | HIGL |
| ATOM | 1772 | CD2 | TYR | 217 | 27.477 | 61.232 | 123.131 | 1.00 | 15.38 | HIGL |
| ATOM | 1773 | CE2 | TYR | 217 | 26.717 | 60.477 | 124.016 | 1.00 | 14.99 | HIGL |
| ATOM | 1774 | CZ | TYR | 217 | 27.324 | 59.875 | 125.102 | 1.00 | 16.23 | HIGL |
| ATOM | 1775 | OH | TYR | 217 | 26.566 | 59.120 | 125.977 | 1.00 | 17.30 | HIGL |
| ATOM | 1776 | C | TYR | 217 | 31.605 | 63.723 | 121.909 | 1.00 | 18.43 | HIGL |
| ATOM | 1777 | O | TYR | 217 | 32.308 | 62.908 | 121.317 | 1.00 | 19.53 | HIGL |
| ATOM | 1778 | N | SER | 218 | 31.693 | 65.034 | 121.703 | 1.00 | 18.33 | HIGL |
| ATOM | 1779 | CA | SER | 218 | 32.616 | 65.598 | 120.724 | 1.00 | 17.79 | HIGL |
| ATOM | 1780 | CB | SER | 218 | 32.501 | 64.839 | 119.403 | 1.00 | 17.69 | HIGL |
| ATOM | 1781 | OG | SER | 218 | 33.128 | 65.542 | 118.347 | 1.00 | 18.59 | HIGL |
| ATOM | 1782 | C | SER | 218 | 32.298 | 67.070 | 120.485 | 1.00 | 17.69 | HIGL |
| ATOM | 1783 | O | SER | 218 | 31.141 | 67.438 | 120.306 | 1.00 | 18.71 | HIGL |
| ATOM | 1784 | N | ALA | 219 | 33.321 | 67.912 | 120.476 | 1.00 | 17.22 | HIGL |
| ATOM | 1785 | CA | ALA | 219 | 33.104 | 69.337 | 120.252 | 1.00 | 17.23 | HIGL |
| ATOM | 1786 | CB | ALA | 219 | 34.382 | 70.118 | 120.554 | 1.00 | 16.44 | HIGL |
| ATOM | 1787 | C | ALA | 219 | 32.661 | 69.589 | 118.816 | 1.00 | 16.60 | HIGL |
| ATOM | 1788 | O | ALA | 219 | 32.258 | 70.696 | 118.467 | 1.00 | 17.34 | HIGL |
| ATOM | 1789 | N | SER | 220 | 32.730 | 68.550 | 117.991 | 1.00 | 16.51 | HIGL |
| ATOM | 1790 | CA | SER | 220 | 32.355 | 68.641 | 116.581 | 1.00 | 16.08 | HIGL |
| ATOM | 1791 | CB | SER | 220 | 32.954 | 67.466 | 115.809 | 1.00 | 15.86 | HIGL |
| ATOM | 1792 | OG | SER | 220 | 34.364 | 67.460 | 115.917 | 1.00 | 16.86 | HIGL |
| ATOM | 1793 | C | SER | 220 | 30.857 | 68.682 | 116.317 | 1.00 | 15.46 | HIGL |
| ATOM | 1794 | O | SER | 220 | 30.432 | 69.049 | 115.229 | 1.00 | 14.91 | HIGL |
| ATOM | 1795 | N | ALA | 221 | 30.061 | 68.300 | 117.309 | 1.00 | 15.99 | HIGL |
| ATOM | 1796 | CA | ALA | 221 | 28.606 | 68.279 | 117.164 | 1.00 | 16.78 | HIGL |
| ATOM | 1797 | CB | ALA | 221 | 27.995 | 67.427 | 118.271 | 1.00 | 16.23 | HIGL |
| ATOM | 1798 | C | ALA | 221 | 27.969 | 69.673 | 117.164 | 1.00 | 17.33 | HIGL |
| ATOM | 1799 | O | ALA | 221 | 27.074 | 69.959 | 117.963 | 1.00 | 17.73 | HIGL |
| ATOM | 1800 | N | THR | 222 | 28.422 | 70.534 | 116.260 | 1.00 | 17.34 | HIGL |
| ATOM | 1801 | CA | THR | 222 | 27.889 | 71.888 | 116.168 | 1.00 | 17.44 | HIGL |
| ATOM | 1802 | CB | THR | 222 | 28.805 | 72.788 | 115.326 | 1.00 | 16.76 | HIGL |
| ATOM | 1803 | OG1 | THR | 222 | 28.859 | 72.290 | 113.988 | 1.00 | 16.54 | HIGL |
| ATOM | 1804 | CG2 | THR | 222 | 30.211 | 72.801 | 115.899 | 1.00 | 17.46 | HIGL |
| ATOM | 1805 | C | THR | 222 | 26.505 | 71.891 | 115.531 | 1.00 | 18.33 | HIGL |
| ATOM | 1806 | O | THR | 222 | 26.189 | 71.044 | 114.692 | 1.00 | 19.58 | HIGL |
| ATOM | 1807 | N | LEU | 223 | 25.675 | 72.842 | 115.933 | 1.00 | 18.21 | HIGL |
| ATOM | 1808 | CA | LEU | 223 | 24.338 | 72.949 | 115.374 | 1.00 | 18.34 | HIGL |
| ATOM | 1809 | CB | LEU | 223 | 23.611 | 74.143 | 115.991 | 1.00 | 18.27 | HIGL |
| ATOM | 1810 | CG | LEU | 223 | 23.370 | 74.045 | 117.500 | 1.00 | 19.89 | HIGL |
| ATOM | 1811 | CD1 | LEU | 223 | 22.888 | 75.388 | 118.034 | 1.00 | 19.53 | HIGL |
| ATOM | 1812 | CD2 | LEU | 223 | 22.340 | 72.943 | 117.786 | 1.00 | 19.06 | HIGL |
| ATOM | 1813 | C | LEU | 223 | 24.437 | 73.122 | 113.860 | 1.00 | 18.82 | HIGL |
| ATOM | 1814 | O | LEU | 223 | 23.605 | 72.608 | 113.120 | 1.00 | 20.15 | HIGL |
| ATOM | 1815 | N | ASP | 224 | 25.457 | 73.846 | 113.406 | 1.00 | 18.59 | HIGL |
| ATOM | 1816 | CA | ASP | 224 | 25.669 | 74.086 | 111.982 | 1.00 | 19.10 | HIGL |
| ATOM | 1817 | CB | ASP | 224 | 26.858 | 75.026 | 111.769 | 1.00 | 18.84 | HIGL |
| ATOM | 1818 | CG | ASP | 224 | 26.468 | 76.494 | 111.816 | 1.00 | 18.91 | HIGL |
| ATOM | 1819 | OD1 | ASP | 224 | 25.286 | 76.812 | 112.069 | 1.00 | 19.14 | HIGL |

# Fig. 2 cont.

| ATOM | 1820 | OD2 | ASP | 224 | 27.355 | 77.341 | 111.593 | 1.00 | 19.90 | HIGL |
|------|------|-----|-----|-----|--------|--------|---------|------|-------|------|
| ATOM | 1821 | C   | ASP | 224 | 25.915 | 72.793 | 111.214 | 1.00 | 19.58 | HIGL |
| ATOM | 1822 | O   | ASP | 224 | 25.341 | 72.583 | 110.146 | 1.00 | 20.23 | HIGL |
| ATOM | 1823 | N   | SER | 225 | 26.785 | 71.939 | 111.750 | 1.00 | 19.67 | HIGL |
| ATOM | 1824 | CA  | SER | 225 | 27.095 | 70.664 | 111.112 | 1.00 | 19.06 | HIGL |
| ATOM | 1825 | CB  | SER | 225 | 28.155 | 69.908 | 111.907 | 1.00 | 18.84 | HIGL |
| ATOM | 1826 | OG  | SER | 225 | 29.403 | 70.567 | 111.840 | 1.00 | 18.91 | HIGL |
| ATOM | 1827 | C   | SER | 225 | 25.838 | 69.811 | 110.997 | 1.00 | 19.40 | HIGL |
| ATOM | 1828 | O   | SER | 225 | 25.601 | 69.186 | 109.968 | 1.00 | 19.64 | HIGL |
| ATOM | 1829 | N   | LEU | 226 | 25.039 | 69.774 | 112.058 | 1.00 | 19.24 | HIGL |
| ATOM | 1830 | CA  | LEU | 226 | 23.799 | 69.009 | 112.026 | 1.00 | 19.90 | HIGL |
| ATOM | 1831 | CB  | LEU | 226 | 23.069 | 69.103 | 113.372 | 1.00 | 18.41 | HIGL |
| ATOM | 1832 | CG  | LEU | 226 | 21.655 | 68.517 | 113.419 | 1.00 | 18.06 | HIGL |
| ATOM | 1833 | CD1 | LEU | 226 | 21.698 | 67.027 | 113.124 | 1.00 | 17.29 | HIGL |
| ATOM | 1834 | CD2 | LEU | 226 | 21.042 | 68.768 | 114.786 | 1.00 | 18.51 | HIGL |
| ATOM | 1835 | C   | LEU | 226 | 22.943 | 69.628 | 110.925 | 1.00 | 20.05 | HIGL |
| ATOM | 1836 | O   | LEU | 226 | 22.369 | 68.932 | 110.086 | 1.00 | 19.89 | HIGL |
| ATOM | 1837 | N   | ARG | 227 | 22.883 | 70.951 | 110.941 | 1.00 | 20.56 | HIGL |
| ATOM | 1838 | CA  | ARG | 227 | 22.127 | 71.717 | 109.965 | 1.00 | 22.15 | HIGL |
| ATOM | 1839 | CB  | ARG | 227 | 22.374 | 73.203 | 110.200 | 1.00 | 23.23 | HIGL |
| ATOM | 1840 | CG  | ARG | 227 | 21.847 | 74.113 | 109.125 | 1.00 | 23.67 | HIGL |
| ATOM | 1841 | CD  | ARG | 227 | 20.585 | 74.801 | 109.561 | 1.00 | 25.35 | HIGL |
| ATOM | 1842 | NE  | ARG | 227 | 20.264 | 75.881 | 108.636 | 1.00 | 27.51 | HIGL |
| ATOM | 1843 | CZ  | ARG | 227 | 20.963 | 77.007 | 108.534 | 1.00 | 27.97 | HIGL |
| ATOM | 1844 | NH1 | ARG | 227 | 22.025 | 77.213 | 109.308 | 1.00 | 27.24 | HIGL |
| ATOM | 1845 | NH2 | ARG | 227 | 20.609 | 77.919 | 107.639 | 1.00 | 28.04 | HIGL |
| ATOM | 1846 | C   | ARG | 227 | 22.532 | 71.349 | 108.541 | 1.00 | 22.77 | HIGL |
| ATOM | 1847 | O   | ARG | 227 | 21.682 | 71.091 | 107.685 | 1.00 | 23.17 | HIGL |
| ATOM | 1848 | N   | ARG | 228 | 23.835 | 71.337 | 108.292 | 1.00 | 22.62 | HIGL |
| ATOM | 1849 | CA  | ARG | 228 | 24.351 | 71.005 | 106.974 | 1.00 | 23.23 | HIGL |
| ATOM | 1850 | CB  | ARG | 228 | 25.854 | 71.275 | 106.907 | 1.00 | 25.19 | HIGL |
| ATOM | 1851 | CG  | ARG | 228 | 26.497 | 70.808 | 105.611 | 1.00 | 27.85 | HIGL |
| ATOM | 1852 | CD  | ARG | 228 | 27.951 | 71.218 | 105.576 | 1.00 | 31.64 | HIGL |
| ATOM | 1853 | NE  | ARG | 228 | 28.217 | 72.426 | 104.784 | 1.00 | 34.16 | HIGL |
| ATOM | 1854 | CZ  | ARG | 228 | 27.482 | 73.539 | 104.787 | 1.00 | 34.92 | HIGL |
| ATOM | 1855 | NH1 | ARG | 228 | 26.385 | 73.644 | 105.537 | 1.00 | 34.00 | HIGL |
| ATOM | 1856 | NH2 | ARG | 228 | 27.869 | 74.572 | 104.049 | 1.00 | 34.79 | HIGL |
| ATOM | 1857 | C   | ARG | 228 | 24.106 | 69.553 | 106.623 | 1.00 | 21.71 | HIGL |
| ATOM | 1858 | O   | ARG | 228 | 23.697 | 69.233 | 105.511 | 1.00 | 21.40 | HIGL |
| ATOM | 1859 | N   | SER | 229 | 24.372 | 68.677 | 107.583 | 1.00 | 20.74 | HIGL |
| ATOM | 1860 | CA  | SER | 229 | 24.209 | 67.248 | 107.385 | 1.00 | 19.19 | HIGL |
| ATOM | 1861 | CB  | SER | 229 | 24.596 | 66.499 | 108.657 | 1.00 | 17.46 | HIGL |
| ATOM | 1862 | OG  | SER | 229 | 24.667 | 65.112 | 108.415 | 1.00 | 16.03 | HIGL |
| ATOM | 1863 | C   | SER | 229 | 22.778 | 66.920 | 106.985 | 1.00 | 19.19 | HIGL |
| ATOM | 1864 | O   | SER | 229 | 22.551 | 66.215 | 106.001 | 1.00 | 19.76 | HIGL |
| ATOM | 1865 | N   | LEU | 230 | 21.816 | 67.443 | 107.738 | 1.00 | 18.51 | HIGL |
| ATOM | 1866 | CA  | LEU | 230 | 20.414 | 67.200 | 107.437 | 1.00 | 18.83 | HIGL |
| ATOM | 1867 | CB  | LEU | 230 | 19.513 | 67.904 | 108.459 | 1.00 | 18.57 | HIGL |
| ATOM | 1868 | CG  | LEU | 230 | 19.748 | 67.471 | 109.906 | 1.00 | 18.99 | HIGL |
| ATOM | 1869 | CD1 | LEU | 230 | 18.765 | 68.159 | 110.830 | 1.00 | 18.90 | HIGL |
| ATOM | 1870 | CD2 | LEU | 230 | 19.611 | 65.966 | 110.011 | 1.00 | 19.09 | HIGL |
| ATOM | 1871 | C   | LEU | 230 | 20.072 | 67.673 | 106.025 | 1.00 | 18.43 | HIGL |
| ATOM | 1872 | O   | LEU | 230 | 19.440 | 66.944 | 105.261 | 1.00 | 18.80 | HIGL |
| ATOM | 1873 | N   | ASN | 231 | 20.492 | 68.887 | 105.678 | 1.00 | 17.99 | HIGL |
| ATOM | 1874 | CA  | ASN | 231 | 20.222 | 69.418 | 104.348 | 1.00 | 18.50 | HIGL |
| ATOM | 1875 | CB  | ASN | 231 | 20.775 | 70.832 | 104.203 | 1.00 | 20.27 | HIGL |
| ATOM | 1876 | CG  | ASN | 231 | 19.831 | 71.884 | 104.755 | 1.00 | 21.88 | HIGL |
| ATOM | 1877 | OD1 | ASN | 231 | 18.703 | 72.029 | 104.276 | 1.00 | 23.81 | HIGL |
| ATOM | 1878 | ND2 | ASN | 231 | 20.284 | 72.624 | 105.763 | 1.00 | 21.50 | HIGL |
| ATOM | 1879 | C   | ASN | 231 | 20.815 | 68.529 | 103.271 | 1.00 | 18.28 | HIGL |
| ATOM | 1880 | O   | ASN | 231 | 20.164 | 68.262 | 102.256 | 1.00 | 17.76 | HIGL |
| ATOM | 1881 | N   | ASN | 232 | 22.042 | 68.064 | 103.497 | 1.00 | 17.66 | HIGL |
| ATOM | 1882 | CA  | ASN | 232 | 22.703 | 67.190 | 102.534 | 1.00 | 17.99 | HIGL |
| ATOM | 1883 | CB  | ASN | 232 | 24.141 | 66.893 | 102.963 | 1.00 | 17.29 | HIGL |
| ATOM | 1884 | CG  | ASN | 232 | 25.037 | 68.116 | 102.915 | 1.00 | 16.38 | HIGL |

# Fig. 2 cont.

| ATOM | 1885 | OD1 | ASN | 232 | 24.686 | 69.141 | 102.334 | 1.00 | 15.50 | HIGL |
|------|------|-----|-----|-----|--------|--------|---------|------|-------|------|
| ATOM | 1886 | ND2 | ASN | 232 | 26.213 | 68.005 | 103.521 | 1.00 | 16.64 | HIGL |
| ATOM | 1887 | C | ASN | 232 | 21.948 | 65.872 | 102.375 | 1.00 | 18.25 | HIGL |
| ATOM | 1888 | O | ASN | 232 | 21.748 | 65.387 | 101.259 | 1.00 | 17.98 | HIGL |
| ATOM | 1889 | N | MET | 233 | 21.536 | 65.298 | 103.501 | 1.00 | 18.52 | HIGL |
| ATOM | 1890 | CA | MET | 233 | 20.805 | 64.033 | 103.507 | 1.00 | 18.43 | HIGL |
| ATOM | 1891 | CB | MET | 233 | 20.538 | 63.589 | 104.951 | 1.00 | 18.18 | HIGL |
| ATOM | 1892 | CG | MET | 233 | 21.795 | 63.269 | 105.754 | 1.00 | 18.25 | HIGL |
| ATOM | 1893 | SD | MET | 233 | 21.474 | 63.063 | 107.531 | 1.00 | 19.43 | HIGL |
| ATOM | 1894 | CE | MET | 233 | 20.199 | 61.766 | 107.504 | 1.00 | 17.54 | HIGL |
| ATOM | 1895 | C | MET | 233 | 19.485 | 64.177 | 102.758 | 1.00 | 18.12 | HIGL |
| ATOM | 1896 | O | MET | 233 | 19.183 | 63.394 | 101.851 | 1.00 | 18.23 | HIGL |
| ATOM | 1897 | N | VAL | 234 | 18.707 | 65.186 | 103.146 | 1.00 | 17.24 | HIGL |
| ATOM | 1898 | CA | VAL | 234 | 17.411 | 65.455 | 102.530 | 1.00 | 16.91 | HIGL |
| ATOM | 1899 | CB | VAL | 234 | 16.744 | 66.687 | 103.179 | 1.00 | 15.88 | HIGL |
| ATOM | 1900 | CG1 | VAL | 234 | 15.486 | 67.056 | 102.420 | 1.00 | 15.35 | HIGL |
| ATOM | 1901 | CG2 | VAL | 234 | 16.413 | 66.390 | 104.638 | 1.00 | 15.47 | HIGL |
| ATOM | 1902 | C | VAL | 234 | 17.502 | 65.678 | 101.017 | 1.00 | 16.63 | HIGL |
| ATOM | 1903 | O | VAL | 234 | 16.784 | 65.045 | 100.245 | 1.00 | 16.27 | HIGL |
| ATOM | 1904 | N | SER | 235 | 18.391 | 66.575 | 100.603 | 1.00 | 16.80 | HIGL |
| ATOM | 1905 | CA | SER | 235 | 18.573 | 66.882 | 99.190 | 1.00 | 17.13 | HIGL |
| ATOM | 1906 | CB | SER | 235 | 19.578 | 68.023 | 99.024 | 1.00 | 17.78 | HIGL |
| ATOM | 1907 | OG | SER | 235 | 19.784 | 68.317 | 97.656 | 1.00 | 17.56 | HIGL |
| ATOM | 1908 | C | SER | 235 | 19.049 | 65.677 | 98.384 | 1.00 | 16.92 | HIGL |
| ATOM | 1909 | O | SER | 235 | 18.768 | 65.562 | 97.190 | 1.00 | 17.15 | HIGL |
| ATOM | 1910 | N | ARG | 236 | 19.759 | 64.774 | 99.045 | 1.00 | 16.40 | HIGL |
| ATOM | 1911 | CA | ARG | 236 | 20.290 | 63.595 | 98.384 | 1.00 | 16.55 | HIGL |
| ATOM | 1912 | CB | ARG | 236 | 21.568 | 63.161 | 99.084 | 1.00 | 17.11 | HIGL |
| ATOM | 1913 | CG | ARG | 236 | 22.156 | 61.872 | 98.562 | 1.00 | 18.73 | HIGL |
| ATOM | 1914 | CD | ARG | 236 | 22.995 | 62.074 | 97.321 | 1.00 | 19.62 | HIGL |
| ATOM | 1915 | NE | ARG | 236 | 23.973 | 60.997 | 97.231 | 1.00 | 24.11 | HIGL |
| ATOM | 1916 | CZ | ARG | 236 | 23.732 | 59.794 | 96.710 | 1.00 | 25.92 | HIGL |
| ATOM | 1917 | NH1 | ARG | 236 | 22.532 | 59.505 | 96.205 | 1.00 | 24.62 | HIGL |
| ATOM | 1918 | NH2 | ARG | 236 | 24.691 | 58.867 | 96.725 | 1.00 | 25.67 | HIGL |
| ATOM | 1919 | C | ARG | 236 | 19.343 | 62.400 | 98.298 | 1.00 | 16.75 | HIGL |
| ATOM | 1920 | O | ARG | 236 | 19.259 | 61.740 | 97.259 | 1.00 | 15.62 | HIGL |
| ATOM | 1921 | N | TRP | 237 | 18.637 | 62.111 | 99.385 | 1.00 | 16.82 | HIGL |
| ATOM | 1922 | CA | TRP | 237 | 17.745 | 60.961 | 99.390 | 1.00 | 16.41 | HIGL |
| ATOM | 1923 | CB | TRP | 237 | 18.224 | 59.966 | 100.453 | 1.00 | 16.05 | HIGL |
| ATOM | 1924 | CG | TRP | 237 | 19.505 | 59.294 | 100.040 | 1.00 | 14.89 | HIGL |
| ATOM | 1925 | CD2 | TRP | 237 | 20.817 | 59.526 | 100.571 | 1.00 | 14.04 | HIGL |
| ATOM | 1926 | CE2 | TRP | 237 | 21.717 | 58.738 | 99.817 | 1.00 | 14.30 | HIGL |
| ATOM | 1927 | CE3 | TRP | 237 | 21.322 | 60.327 | 101.604 | 1.00 | 13.86 | HIGL |
| ATOM | 1928 | CD1 | TRP | 237 | 19.659 | 58.398 | 99.023 | 1.00 | 15.03 | HIGL |
| ATOM | 1929 | NE1 | TRP | 237 | 20.983 | 58.060 | 98.882 | 1.00 | 14.90 | HIGL |
| ATOM | 1930 | CZ2 | TRP | 237 | 23.097 | 58.727 | 100.061 | 1.00 | 13.70 | HIGL |
| ATOM | 1931 | CZ3 | TRP | 237 | 22.695 | 60.319 | 101.847 | 1.00 | 13.61 | HIGL |
| ATOM | 1932 | CH2 | TRP | 237 | 23.566 | 59.522 | 101.074 | 1.00 | 14.26 | HIGL |
| ATOM | 1933 | C | TRP | 237 | 16.266 | 61.281 | 99.557 | 1.00 | 16.86 | HIGL |
| ATOM | 1934 | O | TRP | 237 | 15.430 | 60.383 | 99.522 | 1.00 | 18.12 | HIGL |
| ATOM | 1935 | N | GLY | 238 | 15.953 | 62.562 | 99.732 | 1.00 | 16.74 | HIGL |
| ATOM | 1936 | CA | GLY | 238 | 14.574 | 62.995 | 99.869 | 1.00 | 16.56 | HIGL |
| ATOM | 1937 | C | GLY | 238 | 13.714 | 62.388 | 100.966 | 1.00 | 17.47 | HIGL |
| ATOM | 1938 | O | GLY | 238 | 12.486 | 62.346 | 100.836 | 1.00 | 17.51 | HIGL |
| ATOM | 1939 | N | LYS | 239 | 14.330 | 61.933 | 102.053 | 1.00 | 16.96 | HIGL |
| ATOM | 1940 | CA | LYS | 239 | 13.564 | 61.339 | 103.146 | 1.00 | 16.74 | HIGL |
| ATOM | 1941 | CB | LYS | 239 | 14.327 | 60.152 | 103.724 | 1.00 | 16.66 | HIGL |
| ATOM | 1942 | CG | LYS | 239 | 14.606 | 59.053 | 102.730 | 1.00 | 17.05 | HIGL |
| ATOM | 1943 | CD | LYS | 239 | 13.312 | 58.511 | 102.175 | 1.00 | 15.57 | HIGL |
| ATOM | 1944 | CE | LYS | 239 | 13.561 | 57.342 | 101.262 | 1.00 | 14.83 | HIGL |
| ATOM | 1945 | NZ | LYS | 239 | 12.275 | 56.925 | 100.661 | 1.00 | 14.06 | HIGL |
| ATOM | 1946 | C | LYS | 239 | 13.302 | 62.344 | 104.261 | 1.00 | 16.96 | HIGL |
| ATOM | 1947 | O | LYS | 239 | 14.036 | 63.323 | 104.398 | 1.00 | 17.61 | HIGL |
| ATOM | 1948 | N | GLU | 240 | 12.257 | 62.118 | 105.056 | 1.00 | 17.26 | HIGL |
| ATOM | 1949 | CA | GLU | 240 | 11.985 | 63.016 | 106.181 | 1.00 | 16.82 | HIGL |

# Fig. 2 cont.

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1950 | CB | GLU | 240 | 10.615 | 62.743 | 106.808 | 1.00 | 17.65 | HIGL |
| ATOM | 1951 | CG | GLU | 240 | 9.430 | 63.085 | 105.923 | 1.00 | 18.86 | HIGL |
| ATOM | 1952 | CD | GLU | 240 | 8.116 | 63.080 | 106.690 | 1.00 | 20.65 | HIGL |
| ATOM | 1953 | OE1 | GLU | 240 | 7.818 | 62.067 | 107.353 | 1.00 | 21.31 | HIGL |
| ATOM | 1954 | OE2 | GLU | 240 | 7.381 | 64.091 | 106.634 | 1.00 | 21.43 | HIGL |
| ATOM | 1955 | C | GLU | 240 | 13.088 | 62.751 | 107.209 | 1.00 | 16.31 | HIGL |
| ATOM | 1956 | O | GLU | 240 | 13.562 | 61.621 | 107.360 | 1.00 | 15.76 | HIGL |
| ATOM | 1957 | N | VAL | 241 | 13.493 | 63.793 | 107.917 | 1.00 | 15.69 | HIGL |
| ATOM | 1958 | CA | VAL | 241 | 14.571 | 63.666 | 108.883 | 1.00 | 15.54 | HIGL |
| ATOM | 1959 | CB | VAL | 241 | 15.754 | 64.547 | 108.432 | 1.00 | 14.72 | HIGL |
| ATOM | 1960 | CG1 | VAL | 241 | 16.789 | 64.623 | 109.501 | 1.00 | 17.13 | HIGL |
| ATOM | 1961 | CG2 | VAL | 241 | 16.361 | 63.974 | 107.178 | 1.00 | 15.36 | HIGL |
| ATOM | 1962 | C | VAL | 241 | 14.149 | 64.045 | 110.299 | 1.00 | 15.60 | HIGL |
| ATOM | 1963 | O | VAL | 241 | 13.161 | 64.758 | 110.495 | 1.00 | 16.76 | HIGL |
| ATOM | 1964 | N | ALA | 242 | 14.900 | 63.573 | 111.290 | 1.00 | 14.40 | HIGL |
| ATOM | 1965 | CA | ALA | 242 | 14.577 | 63.888 | 112.673 | 1.00 | 13.72 | HIGL |
| ATOM | 1966 | CB | ALA | 242 | 13.286 | 63.177 | 113.082 | 1.00 | 12.95 | HIGL |
| ATOM | 1967 | C | ALA | 242 | 15.681 | 63.519 | 113.645 | 1.00 | 13.47 | HIGL |
| ATOM | 1968 | O | ALA | 242 | 16.428 | 62.561 | 113.429 | 1.00 | 13.51 | HIGL |
| ATOM | 1969 | N | VAL | 243 | 15.791 | 64.303 | 114.711 | 1.00 | 13.04 | HIGL |
| ATOM | 1970 | CA | VAL | 243 | 16.760 | 64.023 | 115.758 | 1.00 | 13.08 | HIGL |
| ATOM | 1971 | CB | VAL | 243 | 17.192 | 65.294 | 116.497 | 1.00 | 12.64 | HIGL |
| ATOM | 1972 | CG1 | VAL | 243 | 17.918 | 64.924 | 117.771 | 1.00 | 12.23 | HIGL |
| ATOM | 1973 | CG2 | VAL | 243 | 18.088 | 66.125 | 115.604 | 1.00 | 12.08 | HIGL |
| ATOM | 1974 | C | VAL | 243 | 15.964 | 63.139 | 116.701 | 1.00 | 13.56 | HIGL |
| ATOM | 1975 | O | VAL | 243 | 15.014 | 63.593 | 117.346 | 1.00 | 13.37 | HIGL |
| ATOM | 1976 | N | VAL | 244 | 16.328 | 61.866 | 116.754 | 1.00 | 14.00 | HIGL |
| ATOM | 1977 | CA | VAL | 244 | 15.608 | 60.927 | 117.593 | 1.00 | 14.42 | HIGL |
| ATOM | 1978 | CB | VAL | 244 | 15.476 | 59.569 | 116.877 | 1.00 | 13.73 | HIGL |
| ATOM | 1979 | CG1 | VAL | 244 | 14.782 | 59.774 | 115.548 | 1.00 | 13.75 | HIGL |
| ATOM | 1980 | CG2 | VAL | 244 | 16.831 | 58.955 | 116.653 | 1.00 | 12.09 | HIGL |
| ATOM | 1981 | C | VAL | 244 | 16.242 | 60.742 | 118.965 | 1.00 | 15.18 | HIGL |
| ATOM | 1982 | O | VAL | 244 | 15.748 | 59.965 | 119.783 | 1.00 | 14.93 | HIGL |
| ATOM | 1983 | N | GLU | 245 | 17.320 | 61.479 | 119.218 | 1.00 | 15.57 | HIGL |
| ATOM | 1984 | CA | GLU | 245 | 18.023 | 61.397 | 120.490 | 1.00 | 16.66 | HIGL |
| ATOM | 1985 | CB | GLU | 245 | 18.933 | 60.176 | 120.517 | 1.00 | 17.90 | HIGL |
| ATOM | 1986 | CG | GLU | 245 | 18.295 | 58.883 | 120.921 | 1.00 | 19.86 | HIGL |
| ATOM | 1987 | CD | GLU | 245 | 19.325 | 57.778 | 121.021 | 1.00 | 21.19 | HIGL |
| ATOM | 1988 | OE1 | GLU | 245 | 20.395 | 58.018 | 121.624 | 1.00 | 22.19 | HIGL |
| ATOM | 1989 | OE2 | GLU | 245 | 19.071 | 56.673 | 120.502 | 1.00 | 22.22 | HIGL |
| ATOM | 1990 | C | GLU | 245 | 18.892 | 62.616 | 120.780 | 1.00 | 17.25 | HIGL |
| ATOM | 1991 | O | GLU | 245 | 19.756 | 62.984 | 119.979 | 1.00 | 17.63 | HIGL |
| ATOM | 1992 | N | THR | 246 | 18.675 | 63.226 | 121.938 | 1.00 | 16.70 | HIGL |
| ATOM | 1993 | CA | THR | 246 | 19.468 | 64.372 | 122.350 | 1.00 | 16.24 | HIGL |
| ATOM | 1994 | CB | THR | 246 | 19.133 | 65.632 | 121.534 | 1.00 | 16.24 | HIGL |
| ATOM | 1995 | OG1 | THR | 246 | 20.097 | 66.649 | 121.831 | 1.00 | 16.02 | HIGL |
| ATOM | 1996 | CG2 | THR | 246 | 17.737 | 66.146 | 121.872 | 1.00 | 14.97 | HIGL |
| ATOM | 1997 | C | THR | 246 | 19.221 | 64.650 | 123.824 | 1.00 | 16.42 | HIGL |
| ATOM | 1998 | O | THR | 246 | 18.165 | 64.315 | 124.356 | 1.00 | 16.91 | HIGL |
| ATOM | 1999 | N | ASN | 247 | 20.206 | 65.256 | 124.475 | 1.00 | 16.16 | HIGL |
| ATOM | 2000 | CA | ASN | 247 | 20.125 | 65.586 | 125.891 | 1.00 | 16.42 | HIGL |
| ATOM | 2001 | CB | ASN | 247 | 20.753 | 64.482 | 126.754 | 1.00 | 18.32 | HIGL |
| ATOM | 2002 | CG | ASN | 247 | 19.876 | 63.247 | 126.900 | 1.00 | 19.99 | HIGL |
| ATOM | 2003 | OD1 | ASN | 247 | 20.357 | 62.190 | 127.311 | 1.00 | 20.70 | HIGL |
| ATOM | 2004 | ND2 | ASN | 247 | 18.593 | 63.374 | 126.587 | 1.00 | 19.85 | HIGL |
| ATOM | 2005 | C | ASN | 247 | 20.931 | 66.850 | 126.139 | 1.00 | 16.21 | HIGL |
| ATOM | 2006 | O | ASN | 247 | 21.769 | 67.235 | 125.329 | 1.00 | 16.56 | HIGL |
| ATOM | 2007 | N | TRP | 248 | 20.664 | 67.491 | 127.267 | 1.00 | 15.12 | HIGL |
| ATOM | 2008 | CA | TRP | 248 | 21.407 | 68.666 | 127.680 | 1.00 | 14.40 | HIGL |
| ATOM | 2009 | CB | TRP | 248 | 20.750 | 69.965 | 127.235 | 1.00 | 14.05 | HIGL |
| ATOM | 2010 | CG | TRP | 248 | 21.582 | 71.144 | 127.642 | 1.00 | 13.41 | HIGL |
| ATOM | 2011 | CD2 | TRP | 248 | 22.789 | 71.592 | 127.020 | 1.00 | 12.55 | HIGL |
| ATOM | 2012 | CE2 | TRP | 248 | 23.279 | 72.674 | 127.787 | 1.00 | 13.08 | HIGL |
| ATOM | 2013 | CE3 | TRP | 248 | 23.508 | 71.183 | 125.890 | 1.00 | 12.85 | HIGL |
| ATOM | 2014 | CD1 | TRP | 248 | 21.391 | 71.950 | 128.728 | 1.00 | 13.60 | HIGL |

# Fig. 2 cont.

| ATOM | 2015 | NE1 | TRP | 248 | 22.408 | 72.870 | 128.824 | 1.00 | 12.73 | HIGL |
|------|------|-----|-----|-----|--------|--------|---------|------|-------|------|
| ATOM | 2016 | CZ2 | TRP | 248 | 24.457 | 73.352 | 127.458 | 1.00 | 12.54 | HIGL |
| ATOM | 2017 | CZ3 | TRP | 248 | 24.679 | 71.857 | 125.564 | 1.00 | 11.70 | HIGL |
| ATOM | 2018 | CH2 | TRP | 248 | 25.141 | 72.929 | 126.347 | 1.00 | 12.92 | HIGL |
| ATOM | 2019 | C   | TRP | 248 | 21.404 | 68.570 | 129.188 | 1.00 | 14.62 | HIGL |
| ATOM | 2020 | O   | TRP | 248 | 20.351 | 68.434 | 129.802 | 1.00 | 15.22 | HIGL |
| ATOM | 2021 | N   | PRO | 249 | 22.585 | 68.633 | 129.808 | 1.00 | 14.33 | HIGL |
| ATOM | 2022 | CD  | PRO | 249 | 23.925 | 68.623 | 129.197 | 1.00 | 14.04 | HIGL |
| ATOM | 2023 | CA  | PRO | 249 | 22.673 | 68.532 | 131.260 | 1.00 | 14.94 | HIGL |
| ATOM | 2024 | CB  | PRO | 249 | 24.099 | 68.041 | 131.468 | 1.00 | 14.74 | HIGL |
| ATOM | 2025 | CG  | PRO | 249 | 24.836 | 68.752 | 130.390 | 1.00 | 13.70 | HIGL |
| ATOM | 2026 | C   | PRO | 249 | 22.381 | 69.783 | 132.066 | 1.00 | 15.82 | HIGL |
| ATOM | 2027 | O   | PRO | 249 | 22.594 | 70.895 | 131.604 | 1.00 | 16.63 | HIGL |
| ATOM | 2028 | N   | THR | 250 | 21.882 | 69.578 | 133.282 | 1.00 | 17.24 | HIGL |
| ATOM | 2029 | CA  | THR | 250 | 21.603 | 70.672 | 134.207 | 1.00 | 17.83 | HIGL |
| ATOM | 2030 | CB  | THR | 250 | 20.308 | 70.451 | 134.975 | 1.00 | 16.40 | HIGL |
| ATOM | 2031 | OG1 | THR | 250 | 20.478 | 69.353 | 135.875 | 1.00 | 16.53 | HIGL |
| ATOM | 2032 | CG2 | THR | 250 | 19.174 | 70.153 | 134.014 | 1.00 | 17.51 | HIGL |
| ATOM | 2033 | C   | THR | 250 | 22.758 | 70.645 | 135.206 | 1.00 | 18.49 | HIGL |
| ATOM | 2034 | O   | THR | 250 | 22.875 | 71.509 | 136.078 | 1.00 | 19.82 | HIGL |
| ATOM | 2035 | N   | SER | 251 | 23.601 | 69.627 | 135.057 | 1.00 | 18.20 | HIGL |
| ATOM | 2036 | CA  | SER | 251 | 24.769 | 69.426 | 135.897 | 1.00 | 17.27 | HIGL |
| ATOM | 2037 | CB  | SER | 251 | 24.373 | 68.700 | 137.181 | 1.00 | 16.80 | HIGL |
| ATOM | 2038 | OG  | SER | 251 | 25.486 | 68.537 | 138.046 | 1.00 | 16.67 | HIGL |
| ATOM | 2039 | C   | SER | 251 | 25.769 | 68.579 | 135.122 | 1.00 | 17.65 | HIGL |
| ATOM | 2040 | O   | SER | 251 | 25.444 | 67.476 | 134.682 | 1.00 | 17.82 | HIGL |
| ATOM | 2041 | N   | CYS | 252 | 26.975 | 69.099 | 134.936 | 1.00 | 17.77 | HIGL |
| ATOM | 2042 | CA  | CYS | 252 | 28.012 | 68.359 | 134.218 | 1.00 | 19.00 | HIGL |
| ATOM | 2043 | C   | CYS | 252 | 29.375 | 68.791 | 134.751 | 1.00 | 18.46 | HIGL |
| ATOM | 2044 | O   | CYS | 252 | 30.142 | 69.460 | 134.069 | 1.00 | 18.37 | HIGL |
| ATOM | 2045 | CB  | CYS | 252 | 27.940 | 68.611 | 132.703 | 1.00 | 19.48 | HIGL |
| ATOM | 2046 | SG  | CYS | 252 | 28.860 | 67.349 | 131.755 | 1.00 | 21.91 | HIGL |
| ATOM | 2047 | N   | PRO | 253 | 29.687 | 68.402 | 135.992 | 1.00 | 18.43 | HIGL |
| ATOM | 2048 | CD  | PRO | 253 | 28.822 | 67.630 | 136.898 | 1.00 | 17.81 | HIGL |
| ATOM | 2049 | CA  | PRO | 253 | 30.950 | 68.739 | 136.650 | 1.00 | 18.32 | HIGL |
| ATOM | 2050 | CB  | PRO | 253 | 30.789 | 68.130 | 138.038 | 1.00 | 17.88 | HIGL |
| ATOM | 2051 | CG  | PRO | 253 | 29.313 | 68.078 | 138.228 | 1.00 | 18.40 | HIGL |
| ATOM | 2052 | C   | PRO | 253 | 32.191 | 68.204 | 135.952 | 1.00 | 18.83 | HIGL |
| ATOM | 2053 | O   | PRO | 253 | 33.213 | 68.887 | 135.900 | 1.00 | 18.49 | HIGL |
| ATOM | 2054 | N   | TYR | 254 | 32.102 | 66.989 | 135.414 | 1.00 | 19.26 | HIGL |
| ATOM | 2055 | CA  | TYR | 254 | 33.256 | 66.378 | 134.766 | 1.00 | 19.93 | HIGL |
| ATOM | 2056 | CB  | TYR | 254 | 33.782 | 65.223 | 135.616 | 1.00 | 19.85 | HIGL |
| ATOM | 2057 | CG  | TYR | 254 | 33.909 | 65.574 | 137.076 | 1.00 | 19.85 | HIGL |
| ATOM | 2058 | CD1 | TYR | 254 | 32.816 | 65.468 | 137.934 | 1.00 | 18.49 | HIGL |
| ATOM | 2059 | CE1 | TYR | 254 | 32.915 | 65.836 | 139.268 | 1.00 | 18.20 | HIGL |
| ATOM | 2060 | CD2 | TYR | 254 | 35.112 | 66.060 | 137.594 | 1.00 | 19.80 | HIGL |
| ATOM | 2061 | CE2 | TYR | 254 | 35.218 | 66.434 | 138.930 | 1.00 | 18.50 | HIGL |
| ATOM | 2062 | CZ  | TYR | 254 | 34.115 | 66.319 | 139.755 | 1.00 | 18.08 | HIGL |
| ATOM | 2063 | OH  | TYR | 254 | 34.207 | 66.697 | 141.065 | 1.00 | 18.79 | HIGL |
| ATOM | 2064 | C   | TYR | 254 | 33.031 | 65.873 | 133.357 | 1.00 | 21.05 | HIGL |
| ATOM | 2065 | O   | TYR | 254 | 32.995 | 64.667 | 133.128 | 1.00 | 22.11 | HIGL |
| ATOM | 2066 | N   | PRO | 255 | 32.898 | 66.789 | 132.387 | 1.00 | 21.11 | HIGL |
| ATOM | 2067 | CD  | PRO | 255 | 33.042 | 68.251 | 132.488 | 1.00 | 20.35 | HIGL |
| ATOM | 2068 | CA  | PRO | 255 | 32.684 | 66.391 | 130.999 | 1.00 | 21.28 | HIGL |
| ATOM | 2069 | CB  | PRO | 255 | 32.472 | 67.724 | 130.299 | 1.00 | 21.29 | HIGL |
| ATOM | 2070 | CG  | PRO | 255 | 33.369 | 68.632 | 131.075 | 1.00 | 20.00 | HIGL |
| ATOM | 2071 | C   | PRO | 255 | 33.910 | 65.667 | 130.469 | 1.00 | 22.18 | HIGL |
| ATOM | 2072 | O   | PRO | 255 | 35.034 | 66.059 | 130.767 | 1.00 | 22.28 | HIGL |
| ATOM | 2073 | N   | ARG | 256 | 33.698 | 64.613 | 129.686 | 1.00 | 23.41 | HIGL |
| ATOM | 2074 | CA  | ARG | 256 | 34.817 | 63.872 | 129.118 | 1.00 | 24.09 | HIGL |
| ATOM | 2075 | CB  | ARG | 256 | 34.386 | 62.462 | 128.702 | 1.00 | 25.18 | HIGL |
| ATOM | 2076 | CG  | ARG | 256 | 35.537 | 61.602 | 128.198 | 1.00 | 28.36 | HIGL |
| ATOM | 2077 | CD  | ARG | 256 | 35.062 | 60.254 | 127.676 | 1.00 | 31.88 | HIGL |
| ATOM | 2078 | NE  | ARG | 256 | 36.176 | 59.403 | 127.254 | 1.00 | 35.40 | HIGL |
| ATOM | 2079 | CZ  | ARG | 256 | 36.043 | 58.228 | 126.636 | 1.00 | 36.69 | HIGL |

# Fig. 2 cont.

| ATOM | 2080 | NH1 | ARG | 256 | 34.837 | 57.744 | 126.353 | 1.00 | 36.99 | HIGL |
|------|------|-----|-----|-----|--------|--------|---------|------|-------|------|
| ATOM | 2081 | NH2 | ARG | 256 | 37.122 | 57.528 | 126.305 | 1.00 | 37.44 | HIGL |
| ATOM | 2082 | C | ARG | 256 | 35.354 | 64.625 | 127.905 | 1.00 | 23.61 | HIGL |
| ATOM | 2083 | O | ARG | 256 | 36.538 | 64.553 | 127.593 | 1.00 | 23.73 | HIGL |
| ATOM | 2084 | N | TYR | 257 | 34.481 | 65.357 | 127.226 | 1.00 | 22.94 | HIGL |
| ATOM | 2085 | CA | TYR | 257 | 34.893 | 66.107 | 126.054 | 1.00 | 23.27 | HIGL |
| ATOM | 2086 | CB | TYR | 257 | 34.287 | 65.502 | 124.788 | 1.00 | 23.86 | HIGL |
| ATOM | 2087 | CG | TYR | 257 | 34.485 | 64.018 | 124.653 | 1.00 | 24.59 | HIGL |
| ATOM | 2088 | CD1 | TYR | 257 | 33.570 | 63.124 | 125.204 | 1.00 | 25.20 | HIGL |
| ATOM | 2089 | CE1 | TYR | 257 | 33.742 | 61.747 | 125.077 | 1.00 | 26.62 | HIGL |
| ATOM | 2090 | CD2 | TYR | 257 | 35.585 | 63.502 | 123.970 | 1.00 | 24.88 | HIGL |
| ATOM | 2091 | CE2 | TYR | 257 | 35.771 | 62.128 | 123.838 | 1.00 | 26.37 | HIGL |
| ATOM | 2092 | CZ | TYR | 257 | 34.843 | 61.255 | 124.395 | 1.00 | 27.15 | HIGL |
| ATOM | 2093 | OH | TYR | 257 | 35.018 | 59.895 | 124.276 | 1.00 | 27.95 | HIGL |
| ATOM | 2094 | C | TYR | 257 | 34.480 | 67.567 | 126.127 | 1.00 | 23.40 | HIGL |
| ATOM | 2095 | O | TYR | 257 | 33.530 | 67.929 | 126.813 | 1.00 | 23.44 | HIGL |
| ATOM | 2096 | N | GLN | 258 | 35.204 | 68.406 | 125.404 | 1.00 | 23.33 | HIGL |
| ATOM | 2097 | CA | GLN | 258 | 34.886 | 69.816 | 125.367 | 1.00 | 23.32 | HIGL |
| ATOM | 2098 | CB | GLN | 258 | 35.998 | 70.566 | 124.641 | 1.00 | 25.30 | HIGL |
| ATOM | 2099 | CG | GLN | 258 | 35.814 | 72.063 | 124.549 | 1.00 | 29.69 | HIGL |
| ATOM | 2100 | CD | GLN | 258 | 37.146 | 72.781 | 124.380 | 1.00 | 33.22 | HIGL |
| ATOM | 2101 | OE1 | GLN | 258 | 37.199 | 73.936 | 123.943 | 1.00 | 34.85 | HIGL |
| ATOM | 2102 | NE2 | GLN | 258 | 38.234 | 72.099 | 124.741 | 1.00 | 33.71 | HIGL |
| ATOM | 2103 | C | GLN | 258 | 33.573 | 69.922 | 124.608 | 1.00 | 21.85 | HIGL |
| ATOM | 2104 | O | GLN | 258 | 33.359 | 69.209 | 123.632 | 1.00 | 21.62 | HIGL |
| ATOM | 2105 | N | PHE | 259 | 32.680 | 70.784 | 125.067 | 1.00 | 20.74 | HIGL |
| ATOM | 2106 | CA | PHE | 259 | 31.405 | 70.954 | 124.390 | 1.00 | 20.36 | HIGL |
| ATOM | 2107 | CB | PHE | 259 | 30.415 | 71.652 | 125.318 | 1.00 | 20.17 | HIGL |
| ATOM | 2108 | CG | PHE | 259 | 29.691 | 70.718 | 126.243 | 1.00 | 20.50 | HIGL |
| ATOM | 2109 | CD1 | PHE | 259 | 30.383 | 69.756 | 126.969 | 1.00 | 20.48 | HIGL |
| ATOM | 2110 | CD2 | PHE | 259 | 28.310 | 70.803 | 126.391 | 1.00 | 19.48 | HIGL |
| ATOM | 2111 | CE1 | PHE | 259 | 29.707 | 68.887 | 127.830 | 1.00 | 21.21 | HIGL |
| ATOM | 2112 | CE2 | PHE | 259 | 27.629 | 69.943 | 127.246 | 1.00 | 19.74 | HIGL |
| ATOM | 2113 | CZ | PHE | 259 | 28.328 | 68.982 | 127.968 | 1.00 | 20.03 | HIGL |
| ATOM | 2114 | C | PHE | 259 | 31.578 | 71.769 | 123.110 | 1.00 | 20.28 | HIGL |
| ATOM | 2115 | O | PHE | 259 | 32.557 | 72.486 | 122.953 | 1.00 | 19.93 | HIGL |
| ATOM | 2116 | N | PRO | 260 | 30.637 | 71.651 | 122.165 | 1.00 | 20.85 | HIGL |
| ATOM | 2117 | CD | PRO | 260 | 29.527 | 70.687 | 122.073 | 1.00 | 20.21 | HIGL |
| ATOM | 2118 | CA | PRO | 260 | 30.766 | 72.427 | 120.924 | 1.00 | 21.17 | HIGL |
| ATOM | 2119 | CB | PRO | 260 | 29.506 | 72.048 | 120.156 | 1.00 | 21.01 | HIGL |
| ATOM | 2120 | CG | PRO | 260 | 29.291 | 70.617 | 120.584 | 1.00 | 20.56 | HIGL |
| ATOM | 2121 | C | PRO | 260 | 30.837 | 73.928 | 121.239 | 1.00 | 21.74 | HIGL |
| ATOM | 2122 | O | PRO | 260 | 30.163 | 74.414 | 122.150 | 1.00 | 21.19 | HIGL |
| ATOM | 2123 | N | ALA | 261 | 31.657 | 74.654 | 120.487 | 1.00 | 21.93 | HIGL |
| ATOM | 2124 | CA | ALA | 261 | 31.830 | 76.089 | 120.697 | 1.00 | 22.38 | HIGL |
| ATOM | 2125 | CB | ALA | 261 | 32.836 | 76.636 | 119.697 | 1.00 | 21.76 | HIGL |
| ATOM | 2126 | C | ALA | 261 | 30.540 | 76.901 | 120.621 | 1.00 | 22.55 | HIGL |
| ATOM | 2127 | O | ALA | 261 | 30.411 | 77.929 | 121.290 | 1.00 | 23.31 | HIGL |
| ATOM | 2128 | N | ASP | 262 | 29.586 | 76.449 | 119.814 | 1.00 | 22.59 | HIGL |
| ATOM | 2129 | CA | ASP | 262 | 28.331 | 77.173 | 119.674 | 1.00 | 23.66 | HIGL |
| ATOM | 2130 | CB | ASP | 262 | 27.570 | 76.715 | 118.426 | 1.00 | 24.06 | HIGL |
| ATOM | 2131 | CG | ASP | 262 | 27.368 | 75.206 | 118.369 | 1.00 | 25.82 | HIGL |
| ATOM | 2132 | OD1 | ASP | 262 | 27.333 | 74.550 | 119.435 | 1.00 | 26.18 | HIGL |
| ATOM | 2133 | OD2 | ASP | 262 | 27.224 | 74.677 | 117.243 | 1.00 | 26.76 | HIGL |
| ATOM | 2134 | C | ASP | 262 | 27.401 | 77.095 | 120.878 | 1.00 | 24.22 | HIGL |
| ATOM | 2135 | O | ASP | 262 | 26.449 | 77.866 | 120.965 | 1.00 | 24.88 | HIGL |
| ATOM | 2136 | N | VAL | 263 | 27.661 | 76.174 | 121.802 | 1.00 | 25.01 | HIGL |
| ATOM | 2137 | CA | VAL | 263 | 26.803 | 76.042 | 122.976 | 1.00 | 26.27 | HIGL |
| ATOM | 2138 | CB | VAL | 263 | 26.062 | 74.680 | 122.990 | 1.00 | 25.93 | HIGL |
| ATOM | 2139 | CG1 | VAL | 263 | 25.179 | 74.554 | 121.757 | 1.00 | 24.73 | HIGL |
| ATOM | 2140 | CG2 | VAL | 263 | 27.056 | 73.540 | 123.063 | 1.00 | 25.19 | HIGL |
| ATOM | 2141 | C | VAL | 263 | 27.525 | 76.211 | 124.309 | 1.00 | 27.53 | HIGL |
| ATOM | 2142 | O | VAL | 263 | 26.931 | 76.014 | 125.365 | 1.00 | 27.35 | HIGL |
| ATOM | 2143 | N | ARG | 264 | 28.799 | 76.590 | 124.257 | 1.00 | 29.44 | HIGL |
| ATOM | 2144 | CA | ARG | 264 | 29.595 | 76.782 | 125.466 | 1.00 | 31.50 | HIGL |

# Fig. 2 cont.

| ATOM | 2145 | CB | ARG | 264 | 31.066 | 76.969 | 125.092 | 1.00 | 32.75 | HIGL |
|------|------|-----|-----|-----|--------|--------|---------|------|-------|------|
| ATOM | 2146 | CG | ARG | 264 | 31.645 | 75.755 | 124.389 | 1.00 | 35.35 | HIGL |
| ATOM | 2147 | CD | ARG | 264 | 33.075 | 75.968 | 123.917 | 1.00 | 37.11 | HIGL |
| ATOM | 2148 | NE | ARG | 264 | 33.550 | 74.810 | 123.161 | 1.00 | 38.51 | HIGL |
| ATOM | 2149 | CZ | ARG | 264 | 34.738 | 74.727 | 122.571 | 1.00 | 38.26 | HIGL |
| ATOM | 2150 | NH1 | ARG | 264 | 35.590 | 75.742 | 122.646 | 1.00 | 38.84 | HIGL |
| ATOM | 2151 | NH2 | ARG | 264 | 35.072 | 73.629 | 121.903 | 1.00 | 37.21 | HIGL |
| ATOM | 2152 | C | ARG | 264 | 29.110 | 77.968 | 126.294 | 1.00 | 31.82 | HIGL |
| ATOM | 2153 | O | ARG | 264 | 29.649 | 78.256 | 127.360 | 1.00 | 32.57 | HIGL |
| ATOM | 2154 | N | ASN | 265 | 28.086 | 78.648 | 125.796 | 1.00 | 31.94 | HIGL |
| ATOM | 2155 | CA | ASN | 265 | 27.508 | 79.801 | 126.480 | 1.00 | 31.74 | HIGL |
| ATOM | 2156 | CB | ASN | 265 | 27.189 | 80.893 | 125.464 | 1.00 | 33.87 | HIGL |
| ATOM | 2157 | CG | ASN | 265 | 26.419 | 80.357 | 124.264 | 1.00 | 35.62 | HIGL |
| ATOM | 2158 | OD1 | ASN | 265 | 25.213 | 80.600 | 124.115 | 1.00 | 36.81 | HIGL |
| ATOM | 2159 | ND2 | ASN | 265 | 27.113 | 79.608 | 123.407 | 1.00 | 35.24 | HIGL |
| ATOM | 2160 | C | ASN | 265 | 26.227 | 79.376 | 127.175 | 1.00 | 30.26 | HIGL |
| ATOM | 2161 | O | ASN | 265 | 25.738 | 80.064 | 128.067 | 1.00 | 31.10 | HIGL |
| ATOM | 2162 | N | VAL | 266 | 25.685 | 78.240 | 126.746 | 1.00 | 28.31 | HIGL |
| ATOM | 2163 | CA | VAL | 266 | 24.455 | 77.701 | 127.307 | 1.00 | 25.56 | HIGL |
| ATOM | 2164 | CB | VAL | 266 | 23.844 | 76.635 | 126.374 | 1.00 | 25.88 | HIGL |
| ATOM | 2165 | CG1 | VAL | 266 | 22.547 | 76.096 | 126.970 | 1.00 | 25.25 | HIGL |
| ATOM | 2166 | CG2 | VAL | 266 | 23.594 | 77.241 | 124.992 | 1.00 | 24.06 | HIGL |
| ATOM | 2167 | C | VAL | 266 | 24.755 | 77.087 | 128.668 | 1.00 | 23.91 | HIGL |
| ATOM | 2168 | O | VAL | 266 | 25.624 | 76.228 | 128.798 | 1.00 | 23.76 | HIGL |
| ATOM | 2169 | N | PRO | 267 | 24.038 | 77.534 | 129.706 | 1.00 | 21.98 | HIGL |
| ATOM | 2170 | CD | PRO | 267 | 23.034 | 78.615 | 129.662 | 1.00 | 20.37 | HIGL |
| ATOM | 2171 | CA | PRO | 267 | 24.216 | 77.047 | 131.075 | 1.00 | 20.98 | HIGL |
| ATOM | 2172 | CB | PRO | 267 | 23.483 | 78.099 | 131.899 | 1.00 | 20.76 | HIGL |
| ATOM | 2173 | CG | PRO | 267 | 22.349 | 78.475 | 130.996 | 1.00 | 20.01 | HIGL |
| ATOM | 2174 | C | PRO | 267 | 23.670 | 75.655 | 131.340 | 1.00 | 20.67 | HIGL |
| ATOM | 2175 | O | PRO | 267 | 22.759 | 75.190 | 130.652 | 1.00 | 20.51 | HIGL |
| ATOM | 2176 | N | PHE | 268 | 24.239 | 74.985 | 132.338 | 1.00 | 20.18 | HIGL |
| ATOM | 2177 | CA | PHE | 268 | 23.755 | 73.668 | 132.713 | 1.00 | 19.81 | HIGL |
| ATOM | 2178 | CB | PHE | 268 | 24.863 | 72.819 | 133.338 | 1.00 | 19.33 | HIGL |
| ATOM | 2179 | CG | PHE | 268 | 26.001 | 72.540 | 132.405 | 1.00 | 18.57 | HIGL |
| ATOM | 2180 | CD1 | PHE | 268 | 25.755 | 72.175 | 131.079 | 1.00 | 18.00 | HIGL |
| ATOM | 2181 | CD2 | PHE | 268 | 27.320 | 72.663 | 132.837 | 1.00 | 17.98 | HIGL |
| ATOM | 2182 | CE1 | PHE | 268 | 26.802 | 71.941 | 130.196 | 1.00 | 17.94 | HIGL |
| ATOM | 2183 | CE2 | PHE | 268 | 28.382 | 72.431 | 131.961 | 1.00 | 17.83 | HIGL |
| ATOM | 2184 | CZ | PHE | 268 | 28.121 | 72.070 | 130.635 | 1.00 | 18.17 | HIGL |
| ATOM | 2185 | C | PHE | 268 | 22.667 | 73.953 | 133.727 | 1.00 | 19.80 | HIGL |
| ATOM | 2186 | O | PHE | 268 | 22.942 | 74.140 | 134.916 | 1.00 | 19.98 | HIGL |
| ATOM | 2187 | N | SER | 269 | 21.434 | 74.020 | 133.234 | 1.00 | 18.90 | HIGL |
| ATOM | 2188 | CA | SER | 269 | 20.281 | 74.310 | 134.066 | 1.00 | 18.82 | HIGL |
| ATOM | 2189 | CB | SER | 269 | 20.339 | 75.752 | 134.567 | 1.00 | 19.28 | HIGL |
| ATOM | 2190 | OG | SER | 269 | 20.163 | 76.667 | 133.494 | 1.00 | 20.35 | HIGL |
| ATOM | 2191 | C | SER | 269 | 19.021 | 74.133 | 133.243 | 1.00 | 18.90 | HIGL |
| ATOM | 2192 | O | SER | 269 | 19.080 | 73.972 | 132.022 | 1.00 | 19.79 | HIGL |
| ATOM | 2193 | N | ALA | 270 | 17.880 | 74.169 | 133.917 | 1.00 | 17.92 | HIGL |
| ATOM | 2194 | CA | ALA | 270 | 16.604 | 74.030 | 133.245 | 1.00 | 17.69 | HIGL |
| ATOM | 2195 | CB | ALA | 270 | 15.478 | 74.256 | 134.230 | 1.00 | 17.34 | HIGL |
| ATOM | 2196 | C | ALA | 270 | 16.526 | 75.050 | 132.111 | 1.00 | 18.21 | HIGL |
| ATOM | 2197 | O | ALA | 270 | 16.018 | 74.752 | 131.028 | 1.00 | 19.17 | HIGL |
| ATOM | 2198 | N | ALA | 271 | 17.033 | 76.254 | 132.359 | 1.00 | 17.66 | HIGL |
| ATOM | 2199 | CA | ALA | 271 | 17.008 | 77.307 | 131.346 | 1.00 | 16.71 | HIGL |
| ATOM | 2200 | CB | ALA | 271 | 17.545 | 78.605 | 131.926 | 1.00 | 16.21 | HIGL |
| ATOM | 2201 | C | ALA | 271 | 17.838 | 76.886 | 130.145 | 1.00 | 16.17 | HIGL |
| ATOM | 2202 | O | ALA | 271 | 17.407 | 77.035 | 129.006 | 1.00 | 15.94 | HIGL |
| ATOM | 2203 | N | GLY | 272 | 19.024 | 76.348 | 130.415 | 1.00 | 16.09 | HIGL |
| ATOM | 2204 | CA | GLY | 272 | 19.906 | 75.900 | 129.353 | 1.00 | 16.02 | HIGL |
| ATOM | 2205 | C | GLY | 272 | 19.321 | 74.768 | 128.528 | 1.00 | 16.50 | HIGL |
| ATOM | 2206 | O | GLY | 272 | 19.527 | 74.700 | 127.316 | 1.00 | 16.42 | HIGL |
| ATOM | 2207 | N | GLN | 273 | 18.593 | 73.867 | 129.177 | 1.00 | 16.88 | HIGL |
| ATOM | 2208 | CA | GLN | 273 | 17.985 | 72.762 | 128.454 | 1.00 | 17.26 | HIGL |
| ATOM | 2209 | CB | GLN | 273 | 17.267 | 71.809 | 129.414 | 1.00 | 16.57 | HIGL |

# Fig. 2 cont.

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 2210 | CG | GLN | 273 | 18.186 | 71.041 | 130.354 | 1.00 | 16.40 | HIGL |
| ATOM | 2211 | CD | GLN | 273 | 17.438 | 70.007 | 131.175 | 1.00 | 15.47 | HIGL |
| ATOM | 2212 | OE1 | GLN | 273 | 16.479 | 70.330 | 131.868 | 1.00 | 15.89 | HIGL |
| ATOM | 2213 | NE2 | GLN | 273 | 17.877 | 68.758 | 131.101 | 1.00 | 15.09 | HIGL |
| ATOM | 2214 | C | GLN | 273 | 16.986 | 73.323 | 127.452 | 1.00 | 18.10 | HIGL |
| ATOM | 2215 | O | GLN | 273 | 16.955 | 72.903 | 126.297 | 1.00 | 19.02 | HIGL |
| ATOM | 2216 | N | THR | 274 | 16.172 | 74.275 | 127.901 | 1.00 | 18.71 | HIGL |
| ATOM | 2217 | CA | THR | 274 | 15.161 | 74.899 | 127.058 | 1.00 | 19.11 | HIGL |
| ATOM | 2218 | CB | THR | 274 | 14.419 | 76.016 | 127.826 | 1.00 | 20.20 | HIGL |
| ATOM | 2219 | OG1 | THR | 274 | 13.856 | 75.469 | 129.026 | 1.00 | 21.70 | HIGL |
| ATOM | 2220 | CG2 | THR | 274 | 13.293 | 76.603 | 126.978 | 1.00 | 20.14 | HIGL |
| ATOM | 2221 | C | THR | 274 | 15.840 | 75.498 | 125.842 | 1.00 | 19.34 | HIGL |
| ATOM | 2222 | O | THR | 274 | 15.485 | 75.213 | 124.700 | 1.00 | 18.39 | HIGL |
| ATOM | 2223 | N | GLN | 275 | 16.838 | 76.325 | 126.115 | 1.00 | 20.37 | HIGL |
| ATOM | 2224 | CA | GLN | 275 | 17.613 | 76.999 | 125.087 | 1.00 | 21.17 | HIGL |
| ATOM | 2225 | CB | GLN | 275 | 18.747 | 77.761 | 125.766 | 1.00 | 22.42 | HIGL |
| ATOM | 2226 | CG | GLN | 275 | 19.418 | 78.828 | 124.942 | 1.00 | 25.01 | HIGL |
| ATOM | 2227 | CD | GLN | 275 | 20.454 | 79.578 | 125.759 | 1.00 | 28.13 | HIGL |
| ATOM | 2228 | OE1 | GLN | 275 | 20.205 | 79.943 | 126.918 | 1.00 | 28.91 | HIGL |
| ATOM | 2229 | NE2 | GLN | 275 | 21.621 | 79.817 | 125.166 | 1.00 | 29.71 | HIGL |
| ATOM | 2230 | C | GLN | 275 | 18.180 | 75.997 | 124.077 | 1.00 | 21.54 | HIGL |
| ATOM | 2231 | O | GLN | 275 | 18.022 | 76.167 | 122.866 | 1.00 | 21.25 | HIGL |
| ATOM | 2232 | N | TYR | 276 | 18.831 | 74.948 | 124.579 | 1.00 | 20.83 | HIGL |
| ATOM | 2233 | CA | TYR | 276 | 19.431 | 73.941 | 123.712 | 1.00 | 20.67 | HIGL |
| ATOM | 2234 | CB | TYR | 276 | 20.283 | 72.961 | 124.528 | 1.00 | 19.62 | HIGL |
| ATOM | 2235 | CG | TYR | 276 | 20.995 | 71.923 | 123.681 | 1.00 | 18.90 | HIGL |
| ATOM | 2236 | CD1 | TYR | 276 | 22.193 | 72.222 | 123.020 | 1.00 | 18.90 | HIGL |
| ATOM | 2237 | CE1 | TYR | 276 | 22.854 | 71.260 | 122.245 | 1.00 | 18.33 | HIGL |
| ATOM | 2238 | CD2 | TYR | 276· | 20.471 | 70.641 | 123.540 | 1.00 | 18.85 | HIGL |
| ATOM | 2239 | CE2 | TYR | 276 | 21.114 | 69.677 | 122.769 | 1.00 | 18.77 | HIGL |
| ATOM | 2240 | CZ | TYR | 276 | 22.304 | 69.986 | 122.127 | 1.00 | 19.64 | HIGL |
| ATOM | 2241 | OH | TYR | 276 | 22.938 | 69.006 | 121.391 | 1.00 | 19.63 | HIGL |
| ATOM | 2242 | C | TYR | 276 | 18.406 | 73.150 | 122.907 | 1.00 | 20.77 | HIGL |
| ATOM | 2243 | O | TYR | 276 | 18.547 | 72.992 | 121.695 | 1.00 | 20.48 | HIGL |
| ATOM | 2244 | N | ILE | 277 | 17.386 | 72.639 | 123.584 | 1.00 | 21.04 | HIGL |
| ATOM | 2245 | CA | ILE | 277 | 16.361 | 71.857 | 122.912 | 1.00 | 21.46 | HIGL |
| ATOM | 2246 | CB | ILE | 277 | 15.303 | 71.345 | 123.913 | 1.00 | 21.68 | HIGL |
| ATOM | 2247 | CG2 | ILE | 277 | 14.172 | 70.635 | 123.167 | 1.00 | 21.01 | HIGL |
| ATOM | 2248 | CG1 | ILE | 277 | 15.965 | 70.393 | 124.912 | 1.00 | 20.42 | HIGL |
| ATOM | 2249 | CD1 | ILE | 277 | 15.058 | 69.950 | 126.033 | 1.00 | 21.50 | HIGL |
| ATOM | 2250 | C | ILE | 277 | 15.685 | 72.690 | 121.841 | 1.00 | 21.85 | HIGL |
| ATOM | 2251 | O | ILE | 277 | 15.334 | 72.185 | 120.780 | 1.00 | 21.88 | HIGL |
| ATOM | 2252 | N | GLN | 278 | 15.520 | 73.975 | 122.114 | 1.00 | 22.68 | HIGL |
| ATOM | 2253 | CA | GLN | 278 | 14.881 | 74.863 | 121.159 | 1.00 | 23.40 | HIGL |
| ATOM | 2254 | CB | GLN | 278 | 14.468 | 76.164 | 121.856 | 1.00 | 25.27 | HIGL |
| ATOM | 2255 | CG | GLN | 278 | 13.664 | 77.127 | 120.993 | 1.00 | 28.71 | HIGL |
| ATOM | 2256 | CD | GLN | 278 | 12.524 | 77.786 | 121.759 | 1.00 | 31.37 | HIGL |
| ATOM | 2257 | OE1 | GLN | 278 | 12.699 | 78.244 | 122.900 | 1.00 | 32.36 | HIGL |
| ATOM | 2258 | NE2 | GLN | 278 | 11.347 | 77.845 | 121.132 | 1.00 | 31.74 | HIGL |
| ATOM | 2259 | C | GLN | 278 | 15.789 | 75.145 | 119.963 | 1.00 | 22.37 | HIGL |
| ATOM | 2260 | O | GLN | 278 | 15.319 | 75.205 | 118.829 | 1.00 | 22.41 | HIGL |
| ATOM | 2261 | N | SER | 279 | 17.085 | 75.311 | 120.213 | 1.00 | 21.36 | HIGL |
| ATOM | 2262 | CA | SER | 279 | 18.042 | 75.563 | 119.137 | 1.00 | 20.77 | HIGL |
| ATOM | 2263 | CB | SER | 279 | 19.445 | 75.775 | 119.697 | 1.00 | 20.20 | HIGL |
| ATOM | 2264 | OG | SER | 279 | 19.492 | 76.892 | 120.554 | 1.00 | 21.57 | HIGL |
| ATOM | 2265 | C | SER | 279 | 18.083 | 74.372 | 118.185 | 1.00 | 20.98 | HIGL |
| ATOM | 2266 | O | SER | 279 | 18.103 | 74.536 | 116.962 | 1.00 | 21.23 | HIGL |
| ATOM | 2267 | N | VAL | 280 | 18.102 | 73.172 | 118.762 | 1.00 | 20.27 | HIGL |
| ATOM | 2268 | CA | VAL | 280 | 18.141 | 71.945 | 117.983 | 1.00 | 19.59 | HIGL |
| ATOM | 2269 | CB | VAL | 280 | 18.294 | 70.721 | 118.905 | 1.00 | 18.93 | HIGL |
| ATOM | 2270 | CG1 | VAL | 280 | 18.277 | 69.436 | 118.088 | 1.00 | 18.16 | HIGL |
| ATOM | 2271 | CG2 | VAL | 280 | 19.586 | 70.837 | 119.686 | 1.00 | 17.85 | HIGL |
| ATOM | 2272 | C | VAL | 280 | 16.865 | 71.821 | 117.161 | 1.00 | 19.71 | HIGL |
| ATOM | 2273 | O | VAL | 280 | 16.895 | 71.371 | 116.015 | 1.00 | 19.74 | HIGL |
| ATOM | 2274 | N | ALA | 281 | 15.744 | 72.229 | 117.746 | 1.00 | 19.63 | HIGL |

# Fig. 2 cont.

| ATOM | 2275 | CA | ALA | 281 | 14.467 | 72.176 | 117.044 | 1.00 | 19.86 | HIGL |
| ATOM | 2276 | CB | ALA | 281 | 13.324 | 72.570 | 117.982 | 1.00 | 19.49 | HIGL |
| ATOM | 2277 | C | ALA | 281 | 14.519 | 73.123 | 115.847 | 1.00 | 19.99 | HIGL |
| ATOM | 2278 | O | ALA | 281 | 14.070 | 72.782 | 114.751 | 1.00 | 19.99 | HIGL |
| ATOM | 2279 | N | ASN | 282 | 15.080 | 74.309 | 116.056 | 1.00 | 20.40 | HIGL |
| ATOM | 2280 | CA | ASN | 282 | 15.189 | 75.283 | 114.979 | 1.00 | 21.01 | HIGL |
| ATOM | 2281 | CB | ASN | 282 | 15.867 | 76.562 | 115.463 | 1.00 | 22.58 | HIGL |
| ATOM | 2282 | CG | ASN | 282 | 15.081 | 77.253 | 116.555 | 1.00 | 25.95 | HIGL |
| ATOM | 2283 | OD1 | ASN | 282 | 13.850 | 77.335 | 116.489 | 1.00 | 27.58 | HIGL |
| ATOM | 2284 | ND2 | ASN | 282 | 15.786 | 77.765 | 117.567 | 1.00 | 25.99 | HIGL |
| ATOM | 2285 | C | ASN | 282 | 15.976 | 74.709 | 113.818 | 1.00 | 20.44 | HIGL |
| ATOM | 2286 | O | ASN | 282 | 15.608 | 74.915 | 112.662 | 1.00 | 21.36 | HIGL |
| ATOM | 2287 | N | VAL | 283 | 17.058 | 73.995 | 114.118 | 1.00 | 18.69 | HIGL |
| ATOM | 2288 | CA | VAL | 283 | 17.868 | 73.396 | 113.064 | 1.00 | 18.11 | HIGL |
| ATOM | 2289 | CB | VAL | 283 | 19.105 | 72.668 | 113.639 | 1.00 | 17.40 | HIGL |
| ATOM | 2290 | CG1 | VAL | 283 | 19.738 | 71.771 | 112.581 | 1.00 | 15.51 | HIGL |
| ATOM | 2291 | CG2 | VAL | 283 | 20.117 | 73.692 | 114.128 | 1.00 | 15.34 | HIGL |
| ATOM | 2292 | C | VAL | 283 | 17.028 | 72.418 | 112.256 | 1.00 | 18.82 | HIGL |
| ATOM | 2293 | O | VAL | 283 | 16.972 | 72.504 | 111.034 | 1.00 | 19.69 | HIGL |
| ATOM | 2294 | N | VAL | 284 | 16.365 | 71.497 | 112.942 | 1.00 | 19.82 | HIGL |
| ATOM | 2295 | CA | VAL | 284 | 15.518 | 70.514 | 112.277 | 1.00 | 20.48 | HIGL |
| ATOM | 2296 | CB | VAL | 284 | 14.874 | 69.570 | 113.304 | 1.00 | 19.52 | HIGL |
| ATOM | 2297 | CG1 | VAL | 284 | 14.015 | 68.549 | 112.595 | 1.00 | 17.63 | HIGL |
| ATOM | 2298 | CG2 | VAL | 284 | 15.956 | 68.896 | 114.132 | 1.00 | 18.42 | HIGL |
| ATOM | 2299 | C | VAL | 284 | 14.405 | 71.185 | 111.452 | 1.00 | 21.90 | HIGL |
| ATOM | 2300 | O | VAL | 284 | 14.205 | 70.863 | 110.279 | 1.00 | 22.17 | HIGL |
| ATOM | 2301 | N | SER | 285 | 13.685 | 72.117 | 112.068 | 1.00 | 22.19 | HIGL |
| ATOM | 2302 | CA | SER | 285 | 12.609 | 72.820 | 111.380 | 1.00 | 22.67 | HIGL |
| ATOM | 2303 | CB | SER | 285 | 11.936 | 73.817 | 112.317 | 1.00 | 22.73 | HIGL |
| ATOM | 2304 | OG | SER | 285 | 11.369 | 73.153 | 113.426 | 1.00 | 26.28 | HIGL |
| ATOM | 2305 | C | SER | 285 | 13.112 | 73.571 | 110.160 | 1.00 | 23.02 | HIGL |
| ATOM | 2306 | O | SER | 285 | 12.447 | 73.585 | 109.126 | 1.00 | 23.75 | HIGL |
| ATOM | 2307 | N | SER | 286 | 14.279 | 74.203 | 110.282 | 1.00 | 23.31 | HIGL |
| ATOM | 2308 | CA | SER | 286 | 14.848 | 74.975 | 109.177 | 1.00 | 23.26 | HIGL |
| ATOM | 2309 | CB | SER | 286 | 16.231 | 75.524 | 109.545 | 1.00 | 22.79 | HIGL |
| ATOM | 2310 | OG | SER | 286 | 17.224 | 74.513 | 109.479 | 1.00 | 22.57 | HIGL |
| ATOM | 2311 | C | SER | 286 | 14.969 | 74.104 | 107.937 | 1.00 | 23.61 | HIGL |
| ATOM | 2312 | O | SER | 286 | 14.824 | 74.586 | 106.812 | 1.00 | 24.61 | HIGL |
| ATOM | 2313 | N | VAL | 287 | 15.227 | 72.817 | 108.150 | 1.00 | 22.94 | HIGL |
| ATOM | 2314 | CA | VAL | 287 | 15.371 | 71.876 | 107.051 | 1.00 | 22.39 | HIGL |
| ATOM | 2315 | CB | VAL | 287 | 16.126 | 70.596 | 107.494 | 1.00 | 21.12 | HIGL |
| ATOM | 2316 | CG1 | VAL | 287 | 16.217 | 69.617 | 106.341 | 1.00 | 19.58 | HIGL |
| ATOM | 2317 | CG2 | VAL | 287 | 17.500 | 70.952 | 107.989 | 1.00 | 19.96 | HIGL |
| ATOM | 2318 | C | VAL | 287 | 14.020 | 71.452 | 106.510 | 1.00 | 22.70 | HIGL |
| ATOM | 2319 | O | VAL | 287 | 13.129 | 71.075 | 107.266 | 1.00 | 22.82 | HIGL |
| ATOM | 2320 | N | SER | 288 | 13.857 | 71.530 | 105.197 | 1.00 | 23.99 | HIGL |
| ATOM | 2321 | CA | SER | 288 | 12.609 | 71.083 | 104.598 | 1.00 | 25.42 | HIGL |
| ATOM | 2322 | CB | SER | 288 | 12.661 | 71.204 | 103.077 | 1.00 | 25.83 | HIGL |
| ATOM | 2323 | OG | SER | 288 | 13.511 | 70.204 | 102.537 | 1.00 | 26.10 | HIGL |
| ATOM | 2324 | C | SER | 288 | 12.606 | 69.606 | 104.969 | 1.00 | 25.73 | HIGL |
| ATOM | 2325 | O | SER | 288 | 13.655 | 68.951 | 104.917 | 1.00 | 27.44 | HIGL |
| ATOM | 2326 | N | LYS | 289 | 11.456 | 69.073 | 105.342 | 1.00 | 24.12 | HIGL |
| ATOM | 2327 | CA | LYS | 289 | 11.400 | 67.668 | 105.716 | 1.00 | 23.58 | HIGL |
| ATOM | 2328 | CB | LYS | 289 | 12.074 | 66.790 | 104.657 | 1.00 | 23.46 | HIGL |
| ATOM | 2329 | CG | LYS | 289 | 11.229 | 66.659 | 103.407 | 1.00 | 24.42 | HIGL |
| ATOM | 2330 | CD | LYS | 289 | 11.870 | 65.809 | 102.341 | 1.00 | 24.82 | HIGL |
| ATOM | 2331 | CE | LYS | 289 | 10.907 | 65.640 | 101.180 | 1.00 | 25.59 | HIGL |
| ATOM | 2332 | NZ | LYS | 289 | 9.680 | 64.915 | 101.624 | 1.00 | 27.30 | HIGL |
| ATOM | 2333 | C | LYS | 289 | 12.010 | 67.422 | 107.085 | 1.00 | 22.49 | HIGL |
| ATOM | 2334 | O | LYS | 289 | 12.135 | 66.281 | 107.524 | 1.00 | 22.48 | HIGL |
| ATOM | 2335 | N | GLY | 290 | 12.415 | 68.498 | 107.749 | 1.00 | 21.72 | HIGL |
| ATOM | 2336 | CA | GLY | 290 | 12.913 | 68.353 | 109.102 | 1.00 | 21.35 | HIGL |
| ATOM | 2337 | C | GLY | 290 | 11.587 | 68.203 | 109.830 | 1.00 | 20.86 | HIGL |
| ATOM | 2338 | O | GLY | 290 | 10.805 | 69.154 | 109.888 | 1.00 | 21.50 | HIGL |
| ATOM | 2339 | N | VAL | 291 | 11.305 | 67.029 | 110.379 | 1.00 | 19.98 | HIGL |

# Fig. 2 cont.

| ATOM | 2340 | CA  | VAL | 291 | 10.008 | 66.845 | 111.013 | 1.00 | 19.00 | HIGL |
|------|------|-----|-----|-----|--------|--------|---------|------|-------|------|
| ATOM | 2341 | CB  | VAL | 291 | 9.168  | 65.836 | 110.206 | 1.00 | 18.98 | HIGL |
| ATOM | 2342 | CG1 | VAL | 291 | 9.040  | 66.301 | 108.764 | 1.00 | 18.95 | HIGL |
| ATOM | 2343 | CG2 | VAL | 291 | 9.816  | 64.471 | 110.258 | 1.00 | 19.17 | HIGL |
| ATOM | 2344 | C   | VAL | 291 | 9.927  | 66.441 | 112.479 | 1.00 | 18.36 | HIGL |
| ATOM | 2345 | O   | VAL | 291 | 8.834  | 66.482 | 113.055 | 1.00 | 18.16 | HIGL |
| ATOM | 2346 | N   | GLY | 292 | 11.043 | 66.061 | 113.098 | 1.00 | 16.75 | HIGL |
| ATOM | 2347 | CA  | GLY | 292 | 10.943 | 65.657 | 114.489 | 1.00 | 15.82 | HIGL |
| ATOM | 2348 | C   | GLY | 292 | 12.114 | 65.858 | 115.421 | 1.00 | 15.38 | HIGL |
| ATOM | 2349 | O   | GLY | 292 | 13.248 | 66.043 | 114.990 | 1.00 | 15.70 | HIGL |
| ATOM | 2350 | N   | LEU | 293 | 11.822 | 65.825 | 116.719 | 1.00 | 15.28 | HIGL |
| ATOM | 2351 | CA  | LEU | 293 | 12.842 | 65.963 | 117.757 | 1.00 | 14.98 | HIGL |
| ATOM | 2352 | CB  | LEU | 293 | 13.059 | 67.436 | 118.131 | 1.00 | 14.38 | HIGL |
| ATOM | 2353 | CG  | LEU | 293 | 14.200 | 67.697 | 119.131 | 1.00 | 14.97 | HIGL |
| ATOM | 2354 | CD1 | LEU | 293 | 14.507 | 69.175 | 119.180 | 1.00 | 16.01 | HIGL |
| ATOM | 2355 | CD2 | LEU | 293 | 13.824 | 67.197 | 120.524 | 1.00 | 15.85 | HIGL |
| ATOM | 2356 | C   | LEU | 293 | 12.450 | 65.168 | 119.006 | 1.00 | 14.59 | HIGL |
| ATOM | 2357 | O   | LEU | 293 | 11.367 | 65.356 | 119.559 | 1.00 | 14.50 | HIGL |
| ATOM | 2358 | N   | PHE | 294 | 13.334 | 64.281 | 119.454 | 1.00 | 14.69 | HIGL |
| ATOM | 2359 | CA  | PHE | 294 | 13.047 | 63.487 | 120.644 | 1.00 | 14.76 | HIGL |
| ATOM | 2360 | CB  | PHE | 294 | 12.807 | 62.023 | 120.288 | 1.00 | 13.63 | HIGL |
| ATOM | 2361 | CG  | PHE | 294 | 11.566 | 61.788 | 119.496 | 1.00 | 14.32 | HIGL |
| ATOM | 2362 | CD1 | PHE | 294 | 11.557 | 61.983 | 118.116 | 1.00 | 14.42 | HIGL |
| ATOM | 2363 | CD2 | PHE | 294 | 10.394 | 61.372 | 120.127 | 1.00 | 14.49 | HIGL |
| ATOM | 2364 | CE1 | PHE | 294 | 10.395 | 61.763 | 117.372 | 1.00 | 14.13 | HIGL |
| ATOM | 2365 | CE2 | PHE | 294 | 9.225  | 61.149 | 119.397 | 1.00 | 14.10 | HIGL |
| ATOM | 2366 | CZ  | PHE | 294 | 9.224  | 61.344 | 118.017 | 1.00 | 14.44 | HIGL |
| ATOM | 2367 | C   | PHE | 294 | 14.152 | 63.552 | 121.684 | 1.00 | 14.75 | HIGL |
| ATOM | 2368 | O   | PHE | 294 | 15.312 | 63.249 | 121.394 | 1.00 | 15.47 | HIGL |
| ATOM | 2369 | N   | TYR | 295 | 13.778 | 63.947 | 122.897 | 1.00 | 14.13 | HIGL |
| ATOM | 2370 | CA  | TYR | 295 | 14.716 | 64.024 | 124.006 | 1.00 | 13.77 | HIGL |
| ATOM | 2371 | CB  | TYR | 295 | 14.199 | 64.993 | 125.065 | 1.00 | 13.42 | HIGL |
| ATOM | 2372 | CG  | TYR | 295 | 15.267 | 65.439 | 126.031 | 1.00 | 12.18 | HIGL |
| ATOM | 2373 | CD1 | TYR | 295 | 15.972 | 66.628 | 125.825 | 1.00 | 11.42 | HIGL |
| ATOM | 2374 | CE1 | TYR | 295 | 16.991 | 67.020 | 126.696 | 1.00 | 11.09 | HIGL |
| ATOM | 2375 | CD2 | TYR | 295 | 15.602 | 64.656 | 127.131 | 1.00 | 10.29 | HIGL |
| ATOM | 2376 | CE2 | TYR | 295 | 16.612 | 65.040 | 128.004 | 1.00 | 10.79 | HIGL |
| ATOM | 2377 | CZ  | TYR | 295 | 17.304 | 66.217 | 127.782 | 1.00 | 10.57 | HIGL |
| ATOM | 2378 | OH  | TYR | 295 | 18.317 | 66.569 | 128.640 | 1.00 | 9.73  | HIGL |
| ATOM | 2379 | C   | TYR | 295 | 14.783 | 62.609 | 124.586 | 1.00 | 13.63 | HIGL |
| ATOM | 2380 | O   | TYR | 295 | 13.747 | 61.970 | 124.793 | 1.00 | 13.59 | HIGL |
| ATOM | 2381 | N   | TRP | 296 | 15.990 | 62.120 | 124.854 | 1.00 | 12.80 | HIGL |
| ATOM | 2382 | CA  | TRP | 296 | 16.138 | 60.764 | 125.369 | 1.00 | 12.83 | HIGL |
| ATOM | 2383 | CB  | TRP | 296 | 17.412 | 60.119 | 124.809 | 1.00 | 13.03 | HIGL |
| ATOM | 2384 | CG  | TRP | 296 | 17.448 | 58.640 | 125.023 | 1.00 | 13.14 | HIGL |
| ATOM | 2385 | CD2 | TRP | 296 | 18.316 | 57.918 | 125.900 | 1.00 | 13.55 | HIGL |
| ATOM | 2386 | CE2 | TRP | 296 | 17.949 | 56.555 | 125.825 | 1.00 | 13.63 | HIGL |
| ATOM | 2387 | CE3 | TRP | 296 | 19.369 | 58.289 | 126.747 | 1.00 | 14.63 | HIGL |
| ATOM | 2388 | CD1 | TRP | 296 | 16.615 | 57.711 | 124.460 | 1.00 | 14.08 | HIGL |
| ATOM | 2389 | NE1 | TRP | 296 | 16.909 | 56.456 | 124.939 | 1.00 | 13.47 | HIGL |
| ATOM | 2390 | CZ2 | TRP | 296 | 18.596 | 55.562 | 126.567 | 1.00 | 13.78 | HIGL |
| ATOM | 2391 | CZ3 | TRP | 296 | 20.017 | 57.297 | 127.487 | 1.00 | 13.79 | HIGL |
| ATOM | 2392 | CH2 | TRP | 296 | 19.624 | 55.953 | 127.390 | 1.00 | 14.10 | HIGL |
| ATOM | 2393 | C   | TRP | 296 | 16.135 | 60.615 | 126.887 | 1.00 | 12.44 | HIGL |
| ATOM | 2394 | O   | TRP | 296 | 16.964 | 61.202 | 127.582 | 1.00 | 11.79 | HIGL |
| ATOM | 2395 | N   | GLU | 297 | 15.190 | 59.811 | 127.376 | 1.00 | 12.90 | HIGL |
| ATOM | 2396 | CA  | GLU | 297 | 15.029 | 59.502 | 128.797 | 1.00 | 12.94 | HIGL |
| ATOM | 2397 | CB  | GLU | 297 | 16.061 | 58.455 | 129.199 | 1.00 | 13.78 | HIGL |
| ATOM | 2398 | CG  | GLU | 297 | 15.780 | 57.087 | 128.595 | 1.00 | 14.60 | HIGL |
| ATOM | 2399 | CD  | GLU | 297 | 14.616 | 56.394 | 129.271 | 1.00 | 14.61 | HIGL |
| ATOM | 2400 | OE1 | GLU | 297 | 13.947 | 57.031 | 130.112 | 1.00 | 13.68 | HIGL |
| ATOM | 2401 | OE2 | GLU | 297 | 14.370 | 55.211 | 128.962 | 1.00 | 15.38 | HIGL |
| ATOM | 2402 | C   | GLU | 297 | 15.089 | 60.687 | 129.749 | 1.00 | 13.20 | HIGL |
| ATOM | 2403 | O   | GLU | 297 | 15.911 | 60.728 | 130.665 | 1.00 | 11.51 | HIGL |
| ATOM | 2404 | N   | PRO | 298 | 14.185 | 61.659 | 129.563 | 1.00 | 14.35 | HIGL |

# Fig. 2 cont.

| ATOM | 2405 | CD  | PRO | 298 | 13.050 | 61.665 | 128.618 | 1.00 | 14.17 | HIGL |
|------|------|-----|-----|-----|--------|--------|---------|------|-------|------|
| ATOM | 2406 | CA  | PRO | 298 | 14.150 | 62.846 | 130.416 | 1.00 | 14.61 | HIGL |
| ATOM | 2407 | CB  | PRO | 298 | 13.123 | 63.733 | 129.719 | 1.00 | 14.43 | HIGL |
| ATOM | 2408 | CG  | PRO | 298 | 12.143 | 62.727 | 129.206 | 1.00 | 14.48 | HIGL |
| ATOM | 2409 | C   | PRO | 298 | 13.750 | 62.555 | 131.857 | 1.00 | 14.61 | HIGL |
| ATOM | 2410 | O   | PRO | 298 | 14.058 | 63.339 | 132.754 | 1.00 | 15.09 | HIGL |
| ATOM | 2411 | N   | ALA | 299 | 13.082 | 61.427 | 132.080 | 1.00 | 14.64 | HIGL |
| ATOM | 2412 | CA  | ALA | 299 | 12.601 | 61.093 | 133.419 | 1.00 | 15.80 | HIGL |
| ATOM | 2413 | CB  | ALA | 299 | 11.089 | 60.869 | 133.372 | 1.00 | 15.02 | HIGL |
| ATOM | 2414 | C   | ALA | 299 | 13.264 | 59.930 | 134.140 | 1.00 | 16.15 | HIGL |
| ATOM | 2415 | O   | ALA | 299 | 12.746 | 59.459 | 135.148 | 1.00 | 15.99 | HIGL |
| ATOM | 2416 | N   | TRP | 300 | 14.410 | 59.479 | 133.646 | 1.00 | 17.81 | HIGL |
| ATOM | 2417 | CA  | TRP | 300 | 15.115 | 58.361 | 134.269 | 1.00 | 18.35 | HIGL |
| ATOM | 2418 | CB  | TRP | 300 | 16.003 | 57.672 | 133.238 | 1.00 | 17.62 | HIGL |
| ATOM | 2419 | CG  | TRP | 300 | 16.304 | 56.260 | 133.577 | 1.00 | 17.58 | HIGL |
| ATOM | 2420 | CD2 | TRP | 300 | 16.887 | 55.281 | 132.714 | 1.00 | 18.60 | HIGL |
| ATOM | 2421 | CE2 | TRP | 300 | 17.067 | 54.105 | 133.479 | 1.00 | 19.31 | HIGL |
| ATOM | 2422 | CE3 | TRP | 300 | 17.281 | 55.283 | 131.369 | 1.00 | 17.87 | HIGL |
| ATOM | 2423 | CD1 | TRP | 300 | 16.151 | 55.659 | 134.790 | 1.00 | 18.39 | HIGL |
| ATOM | 2424 | NE1 | TRP | 300 | 16.608 | 54.365 | 134.743 | 1.00 | 18.74 | HIGL |
| ATOM | 2425 | CZ2 | TRP | 300 | 17.630 | 52.938 | 132.942 | 1.00 | 19.15 | HIGL |
| ATOM | 2426 | CZ3 | TRP | 300 | 17.843 | 54.123 | 130.835 | 1.00 | 18.15 | HIGL |
| ATOM | 2427 | CH2 | TRP | 300 | 18.011 | 52.969 | 131.621 | 1.00 | 18.86 | HIGL |
| ATOM | 2428 | C   | TRP | 300 | 15.967 | 58.852 | 135.441 | 1.00 | 19.00 | HIGL |
| ATOM | 2429 | O   | TRP | 300 | 17.197 | 58.757 | 135.418 | 1.00 | 19.92 | HIGL |
| ATOM | 2430 | N   | ILE | 301 | 15.299 | 59.358 | 136.473 | 1.00 | 18.81 | HIGL |
| ATOM | 2431 | CA  | ILE | 301 | 15.975 | 59.908 | 137.637 | 1.00 | 18.49 | HIGL |
| ATOM | 2432 | CB  | ILE | 301 | 14.955 | 60.382 | 138.686 | 1.00 | 18.53 | HIGL |
| ATOM | 2433 | CG2 | ILE | 301 | 14.008 | 61.385 | 138.058 | 1.00 | 17.80 | HIGL |
| ATOM | 2434 | CG1 | ILE | 301 | 14.161 | 59.196 | 139.226 | 1.00 | 20.04 | HIGL |
| ATOM | 2435 | CD1 | ILE | 301 | 13.109 | 59.586 | 140.250 | 1.00 | 21.03 | HIGL |
| ATOM | 2436 | C   | ILE | 301 | 17.002 | 59.006 | 138.311 | 1.00 | 18.58 | HIGL |
| ATOM | 2437 | O   | ILE | 301 | 17.991 | 59.499 | 138.851 | 1.00 | 18.75 | HIGL |
| ATOM | 2438 | N   | HIS | 302 | 16.786 | 57.696 | 138.286 | 1.00 | 18.55 | HIGL |
| ATOM | 2439 | CA  | HIS | 302 | 17.741 | 56.781 | 138.907 | 1.00 | 18.79 | HIGL |
| ATOM | 2440 | CB  | HIS | 302 | 17.041 | 55.490 | 139.329 | 1.00 | 18.93 | HIGL |
| ATOM | 2441 | CG  | HIS | 302 | 16.222 | 55.629 | 140.573 | 1.00 | 18.69 | HIGL |
| ATOM | 2442 | CD2 | HIS | 302 | 16.287 | 56.523 | 141.587 | 1.00 | 17.82 | HIGL |
| ATOM | 2443 | ND1 | HIS | 302 | 15.191 | 54.769 | 140.884 | 1.00 | 18.89 | HIGL |
| ATOM | 2444 | CE1 | HIS | 302 | 14.653 | 55.129 | 142.036 | 1.00 | 17.89 | HIGL |
| ATOM | 2445 | NE2 | HIS | 302 | 15.300 | 56.191 | 142.483 | 1.00 | 17.70 | HIGL |
| ATOM | 2446 | C   | HIS | 302 | 18.925 | 56.453 | 137.997 | 1.00 | 19.20 | HIGL |
| ATOM | 2447 | O   | HIS | 302 | 19.703 | 55.542 | 138.289 | 1.00 | 19.21 | HIGL |
| ATOM | 2448 | N   | ASN | 303 | 19.057 | 57.203 | 136.904 | 1.00 | 19.05 | HIGL |
| ATOM | 2449 | CA  | ASN | 303 | 20.140 | 57.013 | 135.944 | 1.00 | 19.03 | HIGL |
| ATOM | 2450 | CB  | ASN | 303 | 19.737 | 55.956 | 134.909 | 1.00 | 19.73 | HIGL |
| ATOM | 2451 | CG  | ASN | 303 | 20.845 | 55.653 | 133.920 | 1.00 | 20.38 | HIGL |
| ATOM | 2452 | OD1 | ASN | 303 | 22.026 | 55.600 | 134.286 | 1.00 | 20.50 | HIGL |
| ATOM | 2453 | ND2 | ASN | 303 | 20.474 | 55.436 | 132.662 | 1.00 | 19.58 | HIGL |
| ATOM | 2454 | C   | ASN | 303 | 20.425 | 58.352 | 135.265 | 1.00 | 19.33 | HIGL |
| ATOM | 2455 | O   | ASN | 303 | 20.706 | 58.413 | 134.068 | 1.00 | 19.13 | HIGL |
| ATOM | 2456 | N   | ALA | 304 | 20.360 | 59.414 | 136.071 | 1.00 | 19.41 | HIGL |
| ATOM | 2457 | CA  | ALA | 304 | 20.562 | 60.804 | 135.654 | 1.00 | 18.77 | HIGL |
| ATOM | 2458 | CB  | ALA | 304 | 20.840 | 61.662 | 136.876 | 1.00 | 17.04 | HIGL |
| ATOM | 2459 | C   | ALA | 304 | 21.603 | 61.102 | 134.584 | 1.00 | 18.84 | HIGL |
| ATOM | 2460 | O   | ALA | 304 | 21.340 | 61.883 | 133.671 | 1.00 | 19.33 | HIGL |
| ATOM | 2461 | N   | ASN | 305 | 22.784 | 60.508 | 134.692 | 1.00 | 19.13 | HIGL |
| ATOM | 2462 | CA  | ASN | 305 | 23.826 | 60.761 | 133.704 | 1.00 | 18.89 | HIGL |
| ATOM | 2463 | CB  | ASN | 305 | 25.162 | 60.163 | 134.158 | 1.00 | 20.60 | HIGL |
| ATOM | 2464 | CG  | ASN | 305 | 25.115 | 58.665 | 134.292 | 1.00 | 21.86 | HIGL |
| ATOM | 2465 | OD1 | ASN | 305 | 24.345 | 58.119 | 135.085 | 1.00 | 23.48 | HIGL |
| ATOM | 2466 | ND2 | ASN | 305 | 25.945 | 57.984 | 133.516 | 1.00 | 23.52 | HIGL |
| ATOM | 2467 | C   | ASN | 305 | 23.448 | 60.207 | 132.343 | 1.00 | 18.26 | HIGL |
| ATOM | 2468 | O   | ASN | 305 | 23.993 | 60.628 | 131.331 | 1.00 | 19.25 | HIGL |
| ATOM | 2469 | N   | LEU | 306 | 22.507 | 59.269 | 132.323 | 1.00 | 17.83 | HIGL |

# Fig. 2 cont.

| ATOM | 2470 | CA  | LEU | 306 | 22.035 | 58.657 | 131.080 | 1.00 | 17.26 | HIGL |
|------|------|-----|-----|-----|--------|--------|---------|------|-------|------|
| ATOM | 2471 | CB  | LEU | 306 | 21.217 | 59.670 | 130.270 | 1.00 | 16.18 | HIGL |
| ATOM | 2472 | CG  | LEU | 306 | 19.907 | 60.128 | 130.937 | 1.00 | 16.97 | HIGL |
| ATOM | 2473 | CD1 | LEU | 306 | 19.284 | 61.278 | 130.161 | 1.00 | 15.17 | HIGL |
| ATOM | 2474 | CD2 | LEU | 306 | 18.937 | 58.954 | 131.024 | 1.00 | 16.01 | HIGL |
| ATOM | 2475 | C   | LEU | 306 | 23.156 | 58.076 | 130.216 | 1.00 | 17.50 | HIGL |
| ATOM | 2476 | O   | LEU | 306 | 23.137 | 58.195 | 128.988 | 1.00 | 17.52 | HIGL |
| ATOM | 2477 | N   | GLY | 307 | 24.131 | 57.450 | 130.870 | 1.00 | 17.26 | HIGL |
| ATOM | 2478 | CA  | GLY | 307 | 25.235 | 56.836 | 130.159 | 1.00 | 16.70 | HIGL |
| ATOM | 2479 | C   | GLY | 307 | 26.294 | 57.773 | 129.616 | 1.00 | 16.64 | HIGL |
| ATOM | 2480 | O   | GLY | 307 | 27.191 | 57.333 | 128.901 | 1.00 | 16.25 | HIGL |
| ATOM | 2481 | N   | SER | 308 | 26.204 | 59.056 | 129.950 | 1.00 | 16.62 | HIGL |
| ATOM | 2482 | CA  | SER | 308 | 27.181 | 60.032 | 129.471 | 1.00 | 17.50 | HIGL |
| ATOM | 2483 | CB  | SER | 308 | 26.477 | 61.300 | 128.987 | 1.00 | 17.40 | HIGL |
| ATOM | 2484 | OG  | SER | 308 | 26.026 | 62.065 | 130.091 | 1.00 | 18.14 | HIGL |
| ATOM | 2485 | C   | SER | 308 | 28.159 | 60.402 | 130.582 | 1.00 | 17.77 | HIGL |
| ATOM | 2486 | O   | SER | 308 | 28.059 | 59.905 | 131.712 | 1.00 | 18.46 | HIGL |
| ATOM | 2487 | N   | SER | 309 | 29.104 | 61.278 | 130.265 | 1.00 | 17.09 | HIGL |
| ATOM | 2488 | CA  | SER | 309 | 30.074 | 61.693 | 131.263 | 1.00 | 17.48 | HIGL |
| ATOM | 2489 | CB  | SER | 309 | 31.384 | 62.138 | 130.599 | 1.00 | 15.98 | HIGL |
| ATOM | 2490 | OG  | SER | 309 | 31.196 | 63.287 | 129.794 | 1.00 | 15.84 | HIGL |
| ATOM | 2491 | C   | SER | 309 | 29.485 | 62.818 | 132.118 | 1.00 | 17.77 | HIGL |
| ATOM | 2492 | O   | SER | 309 | 30.100 | 63.268 | 133.084 | 1.00 | 17.93 | HIGL |
| ATOM | 2493 | N   | CYS | 310 | 28.289 | 63.273 | 131.763 | 1.00 | 18.10 | HIGL |
| ATOM | 2494 | CA  | CYS | 310 | 27.641 | 64.323 | 132.541 | 1.00 | 18.95 | HIGL |
| ATOM | 2495 | C   | CYS | 310 | 26.881 | 63.668 | 133.695 | 1.00 | 18.10 | HIGL |
| ATOM | 2496 | O   | CYS | 310 | 26.437 | 62.528 | 133.583 | 1.00 | 18.94 | HIGL |
| ATOM | 2497 | CB  | CYS | 310 | 26.686 | 65.139 | 131.670 | 1.00 | 19.41 | HIGL |
| ATOM | 2498 | SG  | CYS | 310 | 27.452 | 66.412 | 130.600 | 1.00 | 24.23 | HIGL |
| ATOM | 2499 | N   | ALA | 311 | 26.733 | 64.392 | 134.798 | 1.00 | 16.72 | HIGL |
| ATOM | 2500 | CA  | ALA | 311 | 26.061 | 63.873 | 135.986 | 1.00 | 15.09 | HIGL |
| ATOM | 2501 | CB  | ALA | 311 | 26.451 | 64.713 | 137.187 | 1.00 | 13.34 | HIGL |
| ATOM | 2502 | C   | ALA | 311 | 24.539 | 63.768 | 135.917 | 1.00 | 14.53 | HIGL |
| ATOM | 2503 | O   | ALA | 311 | 23.959 | 62.805 | 136.416 | 1.00 | 14.36 | HIGL |
| ATOM | 2504 | N   | ASP | 312 | 23.893 | 64.755 | 135.308 | 1.00 | 14.02 | HIGL |
| ATOM | 2505 | CA  | ASP | 312 | 22.437 | 64.767 | 135.233 | 1.00 | 14.14 | HIGL |
| ATOM | 2506 | CB  | ASP | 312 | 21.888 | 65.569 | 136.414 | 1.00 | 13.88 | HIGL |
| ATOM | 2507 | CG  | ASP | 312 | 20.417 | 65.338 | 136.647 | 1.00 | 15.05 | HIGL |
| ATOM | 2508 | OD1 | ASP | 312 | 19.703 | 64.943 | 135.692 | 1.00 | 16.00 | HIGL |
| ATOM | 2509 | OD2 | ASP | 312 | 19.973 | 65.562 | 137.795 | 1.00 | 14.74 | HIGL |
| ATOM | 2510 | C   | ASP | 312 | 21.910 | 65.376 | 133.932 | 1.00 | 14.14 | HIGL |
| ATOM | 2511 | O   | ASP | 312 | 22.085 | 66.571 | 133.690 | 1.00 | 13.77 | HIGL |
| ATOM | 2512 | N   | ASN | 313 | 21.260 | 64.555 | 133.108 | 1.00 | 14.50 | HIGL |
| ATOM | 2513 | CA  | ASN | 313 | 20.684 | 65.016 | 131.845 | 1.00 | 15.03 | HIGL |
| ATOM | 2514 | CB  | ASN | 313 | 21.177 | 64.160 | 130.672 | 1.00 | 16.08 | HIGL |
| ATOM | 2515 | CG  | ASN | 313 | 22.633 | 64.403 | 130.337 | 1.00 | 18.13 | HIGL |
| ATOM | 2516 | OD1 | ASN | 313 | 23.069 | 65.544 | 130.228 | 1.00 | 19.71 | HIGL |
| ATOM | 2517 | ND2 | ASN | 313 | 23.391 | 63.326 | 130.159 | 1.00 | 17.96 | HIGL |
| ATOM | 2518 | C   | ASN | 313 | 19.159 | 64.947 | 131.889 | 1.00 | 14.73 | HIGL |
| ATOM | 2519 | O   | ASN | 313 | 18.491 | 65.155 | 130.881 | 1.00 | 14.78 | HIGL |
| ATOM | 2520 | N   | THR | 314 | 18.608 | 64.649 | 133.057 | 1.00 | 15.17 | HIGL |
| ATOM | 2521 | CA  | THR | 314 | 17.160 | 64.535 | 133.207 | 1.00 | 16.32 | HIGL |
| ATOM | 2522 | CB  | THR | 314 | 16.794 | 63.799 | 134.499 | 1.00 | 16.08 | HIGL |
| ATOM | 2523 | OG1 | THR | 314 | 17.198 | 64.596 | 135.619 | 1.00 | 16.57 | HIGL |
| ATOM | 2524 | CG2 | THR | 314 | 17.497 | 62.452 | 134.563 | 1.00 | 15.34 | HIGL |
| ATOM | 2525 | C   | THR | 314 | 16.444 | 65.878 | 133.237 | 1.00 | 16.22 | HIGL |
| ATOM | 2526 | O   | THR | 314 | 17.033 | 66.908 | 133.551 | 1.00 | 17.07 | HIGL |
| ATOM | 2527 | N   | MET | 315 | 15.161 | 65.851 | 132.911 | 1.00 | 16.05 | HIGL |
| ATOM | 2528 | CA  | MET | 315 | 14.352 | 67.055 | 132.929 | 1.00 | 17.30 | HIGL |
| ATOM | 2529 | CB  | MET | 315 | 13.588 | 67.205 | 131.613 | 1.00 | 17.97 | HIGL |
| ATOM | 2530 | CG  | MET | 315 | 14.505 | 67.282 | 130.405 | 1.00 | 18.13 | HIGL |
| ATOM | 2531 | SD  | MET | 315 | 13.637 | 67.606 | 128.894 | 1.00 | 18.76 | HIGL |
| ATOM | 2532 | CE  | MET | 315 | 13.387 | 69.339 | 129.091 | 1.00 | 19.34 | HIGL |
| ATOM | 2533 | C   | MET | 315 | 13.393 | 66.933 | 134.104 | 1.00 | 18.03 | HIGL |
| ATOM | 2534 | O   | MET | 315 | 12.283 | 67.467 | 134.103 | 1.00 | 17.72 | HIGL |

# Fig. 2 cont.

| ATOM | 2535 | N   | PHE | 316 | 13.844 | 66.195 | 135.108 | 1.00 | 18.72 | HIGL |
|------|------|-----|-----|-----|--------|--------|---------|------|-------|------|
| ATOM | 2536 | CA  | PHE | 316 | 13.075 | 66.002 | 136.316 | 1.00 | 19.71 | HIGL |
| ATOM | 2537 | CB  | PHE | 316 | 12.431 | 64.619 | 136.349 | 1.00 | 20.13 | HIGL |
| ATOM | 2538 | CG  | PHE | 316 | 11.179 | 64.517 | 135.541 | 1.00 | 20.75 | HIGL |
| ATOM | 2539 | CD1 | PHE | 316 | 11.232 | 64.450 | 134.153 | 1.00 | 21.09 | HIGL |
| ATOM | 2540 | CD2 | PHE | 316 | 9.942  | 64.492 | 136.167 | 1.00 | 19.49 | HIGL |
| ATOM | 2541 | CE1 | PHE | 316 | 10.065 | 64.359 | 133.402 | 1.00 | 20.74 | HIGL |
| ATOM | 2542 | CE2 | PHE | 316 | 8.776  | 64.401 | 135.429 | 1.00 | 19.68 | HIGL |
| ATOM | 2543 | CZ  | PHE | 316 | 8.836  | 64.335 | 134.041 | 1.00 | 20.74 | HIGL |
| ATOM | 2544 | C   | PHE | 316 | 13.926 | 66.175 | 137.561 | 1.00 | 20.14 | HIGL |
| ATOM | 2545 | O   | PHE | 316 | 15.155 | 66.134 | 137.528 | 1.00 | 21.09 | HIGL |
| ATOM | 2546 | N   | THR | 317 | 13.232 | 66.386 | 138.662 | 1.00 | 20.18 | HIGL |
| ATOM | 2547 | CA  | THR | 317 | 13.836 | 66.550 | 139.960 | 1.00 | 20.01 | HIGL |
| ATOM | 2548 | CB  | THR | 317 | 12.783 | 67.140 | 140.933 | 1.00 | 19.47 | HIGL |
| ATOM | 2549 | OG1 | THR | 317 | 13.102 | 68.508 | 141.196 | 1.00 | 20.10 | HIGL |
| ATOM | 2550 | CG2 | THR | 317 | 12.710 | 66.363 | 142.215 | 1.00 | 18.19 | HIGL |
| ATOM | 2551 | C   | THR | 317 | 14.271 | 65.161 | 140.408 | 1.00 | 20.33 | HIGL |
| ATOM | 2552 | O   | THR | 317 | 13.739 | 64.155 | 139.939 | 1.00 | 20.58 | HIGL |
| ATOM | 2553 | N   | PRO | 318 | 15.265 | 65.087 | 141.299 | 1.00 | 20.32 | HIGL |
| ATOM | 2554 | CD  | PRO | 318 | 16.162 | 66.175 | 141.728 | 1.00 | 20.23 | HIGL |
| ATOM | 2555 | CA  | PRO | 318 | 15.740 | 63.793 | 141.791 | 1.00 | 19.64 | HIGL |
| ATOM | 2556 | CB  | PRO | 318 | 16.859 | 64.187 | 142.743 | 1.00 | 19.58 | HIGL |
| ATOM | 2557 | CG  | PRO | 318 | 17.416 | 65.425 | 142.093 | 1.00 | 19.55 | HIGL |
| ATOM | 2558 | C   | PRO | 318 | 14.615 | 63.044 | 142.498 | 1.00 | 19.76 | HIGL |
| ATOM | 2559 | O   | PRO | 318 | 14.709 | 61.841 | 142.739 | 1.00 | 19.67 | HIGL |
| ATOM | 2560 | N   | SER | 319 | 13.551 | 63.772 | 142.827 | 1.00 | 19.98 | HIGL |
| ATOM | 2561 | CA  | SER | 319 | 12.403 | 63.195 | 143.504 | 1.00 | 20.20 | HIGL |
| ATOM | 2562 | CB  | SER | 319 | 11.887 | 64.147 | 144.578 | 1.00 | 20.64 | HIGL |
| ATOM | 2563 | OG  | SER | 319 | 11.025 | 65.119 | 144.016 | 1.00 | 23.02 | HIGL |
| ATOM | 2564 | C   | SER | 319 | 11.291 | 62.889 | 142.504 | 1.00 | 20.42 | HIGL |
| ATOM | 2565 | O   | SER | 319 | 10.263 | 62.305 | 142.861 | 1.00 | 20.64 | HIGL |
| ATOM | 2566 | N   | GLY | 320 | 11.489 | 63.298 | 141.254 | 1.00 | 20.38 | HIGL |
| ATOM | 2567 | CA  | GLY | 320 | 10.505 | 63.006 | 140.225 | 1.00 | 19.64 | HIGL |
| ATOM | 2568 | C   | GLY | 320 | 9.585  | 64.119 | 139.765 | 1.00 | 19.52 | HIGL |
| ATOM | 2569 | O   | GLY | 320 | 8.657  | 63.862 | 138.996 | 1.00 | 19.02 | HIGL |
| ATOM | 2570 | N   | GLN | 321 | 9.833  | 65.347 | 140.213 | 1.00 | 18.90 | HIGL |
| ATOM | 2571 | CA  | GLN | 321 | 8.991  | 66.475 | 139.824 | 1.00 | 19.06 | HIGL |
| ATOM | 2572 | CB  | GLN | 321 | 8.940  | 67.520 | 140.948 | 1.00 | 20.13 | HIGL |
| ATOM | 2573 | CG  | GLN | 321 | 8.219  | 68.811 | 140.564 | 1.00 | 22.26 | HIGL |
| ATOM | 2574 | CD  | GLN | 321 | 7.946  | 69.703 | 141.762 | 1.00 | 23.01 | HIGL |
| ATOM | 2575 | OE1 | GLN | 321 | 7.346  | 69.264 | 142.748 | 1.00 | 25.05 | HIGL |
| ATOM | 2576 | NE2 | GLN | 321 | 8.377  | 70.958 | 141.682 | 1.00 | 20.98 | HIGL |
| ATOM | 2577 | C   | GLN | 321 | 9.477  | 67.129 | 138.540 | 1.00 | 18.11 | HIGL |
| ATOM | 2578 | O   | GLN | 321 | 10.639 | 67.520 | 138.428 | 1.00 | 17.69 | HIGL |
| ATOM | 2579 | N   | ALA | 322 | 8.578  | 67.263 | 137.574 | 1.00 | 17.71 | HIGL |
| ATOM | 2580 | CA  | ALA | 322 | 8.938  | 67.857 | 136.293 | 1.00 | 17.37 | HIGL |
| ATOM | 2581 | CB  | ALA | 322 | 7.725  | 67.942 | 135.387 | 1.00 | 16.48 | HIGL |
| ATOM | 2582 | C   | ALA | 322 | 9.546  | 69.231 | 136.466 | 1.00 | 17.45 | HIGL |
| ATOM | 2583 | O   | ALA | 322 | 9.078  | 70.041 | 137.268 | 1.00 | 19.09 | HIGL |
| ATOM | 2584 | N   | LEU | 323 | 10.601 | 69.476 | 135.706 | 1.00 | 17.15 | HIGL |
| ATOM | 2585 | CA  | LEU | 323 | 11.305 | 70.743 | 135.720 | 1.00 | 16.94 | HIGL |
| ATOM | 2586 | CB  | LEU | 323 | 12.755 | 70.512 | 135.299 | 1.00 | 16.28 | HIGL |
| ATOM | 2587 | CG  | LEU | 323 | 13.901 | 70.773 | 136.279 | 1.00 | 15.82 | HIGL |
| ATOM | 2588 | CD1 | LEU | 323 | 13.500 | 70.423 | 137.707 | 1.00 | 14.61 | HIGL |
| ATOM | 2589 | CD2 | LEU | 323 | 15.113 | 69.964 | 135.823 | 1.00 | 14.44 | HIGL |
| ATOM | 2590 | C   | LEU | 323 | 10.603 | 71.677 | 134.731 | 1.00 | 17.93 | HIGL |
| ATOM | 2591 | O   | LEU | 323 | 9.883  | 71.225 | 133.838 | 1.00 | 16.70 | HIGL |
| ATOM | 2592 | N   | SER | 324 | 10.811 | 72.980 | 134.893 | 1.00 | 18.92 | HIGL |
| ATOM | 2593 | CA  | SER | 324 | 10.186 | 73.966 | 134.018 | 1.00 | 19.03 | HIGL |
| ATOM | 2594 | CB  | SER | 324 | 10.663 | 75.370 | 134.383 | 1.00 | 19.54 | HIGL |
| ATOM | 2595 | OG  | SER | 324 | 12.069 | 75.478 | 134.241 | 1.00 | 20.56 | HIGL |
| ATOM | 2596 | C   | SER | 324 | 10.496 | 73.707 | 132.555 | 1.00 | 19.19 | HIGL |
| ATOM | 2597 | O   | SER | 324 | 9.628  | 73.843 | 131.697 | 1.00 | 20.39 | HIGL |
| ATOM | 2598 | N   | SER | 325 | 11.743 | 73.338 | 132.282 | 1.00 | 19.12 | HIGL |
| ATOM | 2599 | CA  | SER | 325 | 12.217 | 73.073 | 130.927 | 1.00 | 18.61 | HIGL |

# Fig. 2 cont.

| ATOM | 2600 | CB | SER | 325 | 13.681 | 72.639 | 130.980 | 1.00 | 18.82 | HIGL |
|------|------|-----|-----|-----|--------|--------|---------|------|-------|------|
| ATOM | 2601 | OG | SER | 325 | 13.838 | 71.516 | 131.828 | 1.00 | 18.06 | HIGL |
| ATOM | 2602 | C | SER | 325 | 11.414 | 72.047 | 130.132 | 1.00 | 18.61 | HIGL |
| ATOM | 2603 | O | SER | 325 | 11.458 | 72.036 | 128.905 | 1.00 | 18.45 | HIGL |
| ATOM | 2604 | N | LEU | 326 | 10.680 | 71.184 | 130.820 | 1.00 | 19.28 | HIGL |
| ATOM | 2605 | CA | LEU | 326 | 9.893 | 70.167 | 130.132 | 1.00 | 19.85 | HIGL |
| ATOM | 2606 | CB | LEU | 326 | 9.212 | 69.243 | 131.145 | 1.00 | 20.13 | HIGL |
| ATOM | 2607 | CG | LEU | 326 | 9.112 | 67.733 | 130.862 | 1.00 | 22.13 | HIGL |
| ATOM | 2608 | CD1 | LEU | 326 | 7.849 | 67.179 | 131.542 | 1.00 | 20.56 | HIGL |
| ATOM | 2609 | CD2 | LEU | 326 | 9.063 | 67.453 | 129.364 | 1.00 | 21.71 | HIGL |
| ATOM | 2610 | C | LEU | 326 | 8.822 | 70.787 | 129.230 | 1.00 | 20.36 | HIGL |
| ATOM | 2611 | O | LEU | 326 | 8.415 | 70.187 | 128.233 | 1.00 | 19.41 | HIGL |
| ATOM | 2612 | N | SER | 327 | 8.363 | 71.986 | 129.580 | 1.00 | 20.97 | HIGL |
| ATOM | 2613 | CA | SER | 327 | 7.317 | 72.642 | 128.803 | 1.00 | 21.71 | HIGL |
| ATOM | 2614 | CB | SER | 327 | 6.595 | 73.684 | 129.653 | 1.00 | 21.54 | HIGL |
| ATOM | 2615 | OG | SER | 327 | 7.439 | 74.785 | 129.921 | 1.00 | 23.10 | HIGL |
| ATOM | 2616 | C | SER | 327 | 7.829 | 73.301 | 127.533 | 1.00 | 22.18 | HIGL |
| ATOM | 2617 | O | SER | 327 | 7.100 | 74.056 | 126.887 | 1.00 | 23.13 | HIGL |
| ATOM | 2618 | N | VAL | 328 | 9.080 | 73.032 | 127.180 | 1.00 | 21.90 | HIGL |
| ATOM | 2619 | CA | VAL | 328 | 9.651 | 73.588 | 125.959 | 1.00 | 22.31 | HIGL |
| ATOM | 2620 | CB | VAL | 328 | 11.188 | 73.333 | 125.873 | 1.00 | 22.21 | HIGL |
| ATOM | 2621 | CG1 | VAL | 328 | 11.483 | 71.843 | 125.809 | 1.00 | 21.74 | HIGL |
| ATOM | 2622 | CG2 | VAL | 328 | 11.759 | 74.026 | 124.657 | 1.00 | 21.78 | HIGL |
| ATOM | 2623 | C | VAL | 328 | 8.958 | 72.917 | 124.764 | 1.00 | 22.65 | HIGL |
| ATOM | 2624 | O | VAL | 328 | 8.973 | 73.429 | 123.645 | 1.00 | 22.63 | HIGL |
| ATOM | 2625 | N | PHE | 329 | 8.338 | 71.771 | 125.013 | 1.00 | 22.73 | HIGL |
| ATOM | 2626 | CA | PHE | 329 | 7.654 | 71.048 | 123.959 | 1.00 | 23.91 | HIGL |
| ATOM | 2627 | CB | PHE | 329 | 7.268 | 69.658 | 124.454 | 1.00 | 23.67 | HIGL |
| ATOM | 2628 | CG | PHE | 329 | 8.440 | 68.723 | 124.557 | 1.00 | 24.39 | HIGL |
| ATOM | 2629 | CD1 | PHE | 329 | 9.067 | 68.252 | 123.409 | 1.00 | 24.10 | HIGL |
| ATOM | 2630 | CD2 | PHE | 329 | 8.949 | 68.349 | 125.796 | 1.00 | 23.95 | HIGL |
| ATOM | 2631 | CE1 | PHE | 329 | 10.185 | 67.424 | 123.491 | 1.00 | 24.86 | HIGL |
| ATOM | 2632 | CE2 | PHE | 329 | 10.063 | 67.524 | 125.887 | 1.00 | 24.79 | HIGL |
| ATOM | 2633 | CZ | PHE | 329 | 10.686 | 67.060 | 124.729 | 1.00 | 24.99 | HIGL |
| ATOM | 2634 | C | PHE | 329 | 6.446 | 71.806 | 123.420 | 1.00 | 24.94 | HIGL |
| ATOM | 2635 | O | PHE | 329 | 5.885 | 71.438 | 122.384 | 1.00 | 24.54 | HIGL |
| ATOM | 2636 | N | HIS | 330 | 6.053 | 72.867 | 124.123 | 1.00 | 25.53 | HIGL |
| ATOM | 2637 | CA | HIS | 330 | 4.944 | 73.706 | 123.677 | 1.00 | 25.92 | HIGL |
| ATOM | 2638 | CB | HIS | 330 | 4.376 | 74.554 | 124.828 | 1.00 | 25.05 | HIGL |
| ATOM | 2639 | CG | HIS | 330 | 3.507 | 73.795 | 125.786 | 1.00 | 23.98 | HIGL |
| ATOM | 2640 | CD2 | HIS | 330 | 3.511 | 73.739 | 127.139 | 1.00 | 23.72 | HIGL |
| ATOM | 2641 | ND1 | HIS | 330 | 2.451 | 73.010 | 125.377 | 1.00 | 23.63 | HIGL |
| ATOM | 2642 | CE1 | HIS | 330 | 1.843 | 72.503 | 126.434 | 1.00 | 22.96 | HIGL |
| ATOM | 2643 | NE2 | HIS | 330 | 2.467 | 72.931 | 127.517 | 1.00 | 23.30 | HIGL |
| ATOM | 2644 | C | HIS | 330 | 5.488 | 74.650 | 122.601 | 1.00 | 26.65 | HIGL |
| ATOM | 2645 | O | HIS | 330 | 4.891 | 74.806 | 121.540 | 1.00 | 27.30 | HIGL |
| ATOM | 2646 | N | ARG | 331 | 6.632 | 75.267 | 122.888 | 1.00 | 27.80 | HIGL |
| ATOM | 2647 | CA | ARG | 331 | 7.273 | 76.214 | 121.976 | 1.00 | 28.68 | HIGL |
| ATOM | 2648 | CB | ARG | 331 | 8.405 | 76.953 | 122.698 | 1.00 | 31.32 | HIGL |
| ATOM | 2649 | CG | ARG | 331 | 7.935 | 78.120 | 123.555 | 1.00 | 35.13 | HIGL |
| ATOM | 2650 | CD | ARG | 331 | 9.101 | 78.976 | 124.057 | 1.00 | 37.60 | HIGL |
| ATOM | 2651 | NE | ARG | 331 | 9.862 | 78.322 | 125.116 | 1.00 | 39.32 | HIGL |
| ATOM | 2652 | CZ | ARG | 331 | 9.311 | 77.800 | 126.208 | 1.00 | 41.08 | HIGL |
| ATOM | 2653 | NH1 | ARG | 331 | 7.994 | 77.854 | 126.382 | 1.00 | 41.70 | HIGL |
| ATOM | 2654 | NH2 | ARG | 331 | 10.075 | 77.233 | 127.133 | 1.00 | 41.35 | HIGL |
| ATOM | 2655 | C | ARG | 331 | 7.821 | 75.668 | 120.661 | 1.00 | 28.01 | HIGL |
| ATOM | 2656 | O | ARG | 331 | 8.119 | 76.440 | 119.753 | 1.00 | 28.33 | HIGL |
| ATOM | 2657 | N | ILE | 332 | 7.966 | 74.355 | 120.545 | 1.00 | 27.15 | HIGL |
| ATOM | 2658 | CA | ILE | 332 | 8.503 | 73.790 | 119.313 | 1.00 | 25.82 | HIGL |
| ATOM | 2659 | CB | ILE | 332 | 9.717 | 72.876 | 119.596 | 1.00 | 24.07 | HIGL |
| ATOM | 2660 | CG2 | ILE | 332 | 10.747 | 73.636 | 120.419 | 1.00 | 22.61 | HIGL |
| ATOM | 2661 | CG1 | ILE | 332 | 9.262 | 71.611 | 120.331 | 1.00 | 23.55 | HIGL |
| ATOM | 2662 | CD1 | ILE | 332 | 10.328 | 70.559 | 120.487 | 1.00 | 21.73 | HIGL |
| ATOM | 2663 | C | ILE | 332 | 7.463 | 72.999 | 118.534 | 1.00 | 26.35 | HIGL |
| ATOM | 2664 | O | ILE | 332 | 7.659 | 72.716 | 117.351 | 1.00 | 27.46 | HIGL |
| END | | | | | | | | | | |

# Fig. 2 cont.

| HEADER | | | | | | | | | | AAGL |
|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1 | CB | ALA | 1 | 30.233 | 36.166 | 100.975 | 1.00 | 33.89 | AAGL |
| ATOM | 2 | C | ALA | 1 | 30.173 | 35.826 | 103.455 | 1.00 | 33.23 | AAGL |
| ATOM | 3 | O | ALA | 1 | 30.978 | 35.045 | 103.960 | 1.00 | 32.69 | AAGL |
| ATOM | 4 | N | ALA | 1 | 32.066 | 36.993 | 102.404 | 1.00 | 32.99 | AAGL |
| ATOM | 5 | CA | ALA | 1 | 30.595 | 36.767 | 102.330 | 1.00 | 33.73 | AAGL |
| ATOM | 6 | N | LEU | 2 | 28.909 | 35.906 | 103.856 | 1.00 | 31.18 | AAGL |
| ATOM | 7 | CA | LEU | 2 | 28.412 | 35.052 | 104.926 | 1.00 | 29.30 | AAGL |
| ATOM | 8 | CB | LEU | 2 | 27.023 | 35.510 | 105.362 | 1.00 | 29.79 | AAGL |
| ATOM | 9 | CG | LEU | 2 | 26.868 | 36.944 | 105.864 | 1.00 | 30.10 | AAGL |
| ATOM | 10 | CD1 | LEU | 2 | 25.382 | 37.292 | 105.912 | 1.00 | 32.47 | AAGL |
| ATOM | 11 | CD2 | LEU | 2 | 27.511 | 37.098 | 107.236 | 1.00 | 30.25 | AAGL |
| ATOM | 12 | C | LEU | 2 | 28.340 | 33.612 | 104.451 | 1.00 | 28.19 | AAGL |
| ATOM | 13 | O | LEU | 2 | 28.258 | 33.351 | 103.250 | 1.00 | 28.93 | AAGL |
| ATOM | 14 | N | THR | 3 | 28.370 | 32.679 | 105.396 | 1.00 | 27.70 | AAGL |
| ATOM | 15 | CA | THR | 3 | 28.304 | 31.267 | 105.071 | 1.00 | 27.25 | AAGL |
| ATOM | 16 | CB | THR | 3 | 28.401 | 30.410 | 106.349 | 1.00 | 28.42 | AAGL |
| ATOM | 17 | OG1 | THR | 3 | 29.650 | 30.681 | 107.001 | 1.00 | 28.17 | AAGL |
| ATOM | 18 | CG2 | THR | 3 | 28.327 | 28.920 | 106.010 | 1.00 | 27.90 | AAGL |
| ATOM | 19 | C | THR | 3 | 27.000 | 30.971 | 104.343 | 1.00 | 26.98 | AAGL |
| ATOM | 20 | O | THR | 3 | 26.965 | 30.159 | 103.416 | 1.00 | 26.10 | AAGL |
| ATOM | 21 | N | TYR | 4 | 25.931 | 31.650 | 104.756 | 1.00 | 26.84 | AAGL |
| ATOM | 22 | CA | TYR | 4 | 24.623 | 31.465 | 104.137 | 1.00 | 24.81 | AAGL |
| ATOM | 23 | CB | TYR | 4 | 23.665 | 30.721 | 105.079 | 1.00 | 25.74 | AAGL |
| ATOM | 24 | CG | TYR | 4 | 24.137 | 29.377 | 105.602 | 1.00 | 25.74 | AAGL |
| ATOM | 25 | CD1 | TYR | 4 | 24.318 | 28.288 | 104.746 | 1.00 | 26.33 | AAGL |
| ATOM | 26 | CE1 | TYR | 4 | 24.692 | 27.034 | 105.247 | 1.00 | 27.71 | AAGL |
| ATOM | 27 | CD2 | TYR | 4 | 24.349 | 29.182 | 106.965 | 1.00 | 25.74 | AAGL |
| ATOM | 28 | CE2 | TYR | 4 | 24.724 | 27.940 | 107.473 | 1.00 | 26.87 | AAGL |
| ATOM | 29 | CZ | TYR | 4 | 24.891 | 26.870 | 106.609 | 1.00 | 26.22 | AAGL |
| ATOM | 30 | OH | TYR | 4 | 25.248 | 25.646 | 107.118 | 1.00 | 29.24 | AAGL |
| ATOM | 31 | C | TYR | 4 | 23.977 | 32.803 | 103.787 | 1.00 | 24.69 | AAGL |
| ATOM | 32 | O | TYR | 4 | 23.914 | 33.712 | 104.619 | 1.00 | 24.65 | AAGL |
| ATOM | 33 | N | ARG | 5 | 23.515 | 32.919 | 102.549 | 1.00 | 23.45 | AAGL |
| ATOM | 34 | CA | ARG | 5 | 22.801 | 34.103 | 102.069 | 1.00 | 25.24 | AAGL |
| ATOM | 35 | CB | ARG | 5 | 23.551 | 34.823 | 100.939 | 1.00 | 29.22 | AAGL |
| ATOM | 36 | CG | ARG | 5 | 24.781 | 35.609 | 101.366 | 1.00 | 29.88 | AAGL |
| ATOM | 37 | CD | ARG | 5 | 26.042 | 34.797 | 101.168 | 1.00 | 29.48 | AAGL |
| ATOM | 38 | NE | ARG | 5 | 26.159 | 34.336 | 99.792 | 1.00 | 29.78 | AAGL |
| ATOM | 39 | CZ | ARG | 5 | 27.061 | 33.454 | 99.373 | 1.00 | 27.81 | AAGL |
| ATOM | 40 | NH1 | ARG | 5 | 27.934 | 32.940 | 100.225 | 1.00 | 27.49 | AAGL |
| ATOM | 41 | NH2 | ARG | 5 | 27.068 | 33.068 | 98.104 | 1.00 | 29.30 | AAGL |
| ATOM | 42 | C | ARG | 5 | 21.554 | 33.439 | 101.507 | 1.00 | 25.34 | AAGL |
| ATOM | 43 | O | ARG | 5 | 21.547 | 32.962 | 100.371 | 1.00 | 23.77 | AAGL |
| ATOM | 44 | N | GLY | 6 | 20.502 | 33.381 | 102.308 | 1.00 | 24.34 | AAGL |
| ATOM | 45 | CA | GLY | 6 | 19.321 | 32.694 | 101.837 | 1.00 | 21.41 | AAGL |
| ATOM | 46 | C | GLY | 6 | 18.031 | 33.457 | 101.755 | 1.00 | 22.93 | AAGL |
| ATOM | 47 | O | GLY | 6 | 17.957 | 34.649 | 102.053 | 1.00 | 21.36 | AAGL |
| ATOM | 48 | N | ALA | 7 | 17.008 | 32.727 | 101.330 | 1.00 | 21.72 | AAGL |
| ATOM | 49 | CA | ALA | 7 | 15.669 | 33.248 | 101.182 | 1.00 | 22.02 | AAGL |
| ATOM | 50 | CB | ALA | 7 | 15.481 | 33.797 | 99.780 | 1.00 | 22.89 | AAGL |
| ATOM | 51 | C | ALA | 7 | 14.689 | 32.110 | 101.422 | 1.00 | 21.79 | AAGL |
| ATOM | 52 | O | ALA | 7 | 14.973 | 30.956 | 101.101 | 1.00 | 23.27 | AAGL |
| ATOM | 53 | N | ASP | 8 | 13.548 | 32.435 | 102.014 | 1.00 | 20.87 | AAGL |
| ATOM | 54 | CA | ASP | 8 | 12.501 | 31.448 | 102.247 | 1.00 | 21.47 | AAGL |
| ATOM | 55 | CB | ASP | 8 | 11.854 | 31.650 | 103.625 | 1.00 | 20.38 | AAGL |
| ATOM | 56 | CG | ASP | 8 | 10.772 | 30.617 | 103.923 | 1.00 | 20.93 | AAGL |
| ATOM | 57 | OD1 | ASP | 8 | 9.920 | 30.363 | 103.044 | 1.00 | 20.43 | AAGL |
| ATOM | 58 | OD2 | ASP | 8 | 10.768 | 30.069 | 105.048 | 1.00 | 19.51 | AAGL |
| ATOM | 59 | C | ASP | 8 | 11.482 | 31.736 | 101.153 | 1.00 | 19.96 | AAGL |
| ATOM | 60 | O | ASP | 8 | 10.773 | 32.738 | 101.205 | 1.00 | 21.04 | AAGL |
| ATOM | 61 | N | ILE | 9 | 11.424 | 30.870 | 100.149 | 1.00 | 20.91 | AAGL |
| ATOM | 62 | CA | ILE | 9 | 10.490 | 31.065 | 99.049 | 1.00 | 21.73 | AAGL |
| ATOM | 63 | CB | ILE | 9 | 11.234 | 31.102 | 97.689 | 1.00 | 21.80 | AAGL |
| ATOM | 64 | CG2 | ILE | 9 | 12.174 | 32.300 | 97.648 | 1.00 | 23.18 | AAGL |
| ATOM | 65 | CG1 | ILE | 9 | 12.015 | 29.807 | 97.479 | 1.00 | 22.70 | AAGL |

# Fig. 3

| ATOM | 66 | CD1 | ILE | 9 | 12.626 | 29.683 | 96.085 | 1.00 | 25.10 | AAGL |
|------|-----|-----|-----|----|--------|--------|---------|------|-------|------|
| ATOM | 67 | C | ILE | 9 | 9.452 | 29.945 | 99.038 | 1.00 | 23.69 | AAGL |
| ATOM | 68 | O | ILE | 9 | 9.018 | 29.490 | 97.984 | 1.00 | 22.97 | AAGL |
| ATOM | 69 | N | SER | 10 | 9.059 | 29.511 | 100.232 | 1.00 | 22.26 | AAGL |
| ATOM | 70 | CA | SER | 10 | 8.080 | 28.441 | 100.377 | 1.00 | 22.83 | AAGL |
| ATOM | 71 | CB | SER | 10 | 7.658 | 28.325 | 101.840 | 1.00 | 20.03 | AAGL |
| ATOM | 72 | OG | SER | 10 | 8.782 | 28.078 | 102.658 | 1.00 | 21.43 | AAGL |
| ATOM | 73 | C | SER | 10 | 6.833 | 28.617 | 99.508 | 1.00 | 22.20 | AAGL |
| ATOM | 74 | O | SER | 10 | 6.286 | 27.649 | 98.995 | 1.00 | 24.50 | AAGL |
| ATOM | 75 | N | SER | 11 | 6.388 | 29.855 | 99.347 | 1.00 | 23.05 | AAGL |
| ATOM | 76 | CA | SER | 11 | 5.198 | 30.148 | 98.563 | 1.00 | 24.59 | AAGL |
| ATOM | 77 | CB | SER | 11 | 4.784 | 31.598 | 98.792 | 1.00 | 26.58 | AAGL |
| ATOM | 78 | OG | SER | 11 | 5.775 | 32.473 | 98.275 | 1.00 | 26.05 | AAGL |
| ATOM | 79 | C | SER | 11 | 5.347 | 29.935 | 97.057 | 1.00 | 25.49 | AAGL |
| ATOM | 80 | O | SER | 11 | 4.351 | 29.913 | 96.338 | 1.00 | 25.69 | AAGL |
| ATOM | 81 | N | LEU | 12 | 6.578 | 29.781 | 96.583 | 1.00 | 26.51 | AAGL |
| ATOM | 82 | CA | LEU | 12 | 6.817 | 29.637 | 95.149 | 1.00 | 25.87 | AAGL |
| ATOM | 83 | CB | LEU | 12 | 8.237 | 29.143 | 94.884 | 1.00 | 26.84 | AAGL |
| ATOM | 84 | CG | LEU | 12 | 8.609 | 29.025 | 93.398 | 1.00 | 26.26 | AAGL |
| ATOM | 85 | CD1 | LEU | 12 | 8.307 | 30.324 | 92.665 | 1.00 | 26.19 | AAGL |
| ATOM | 86 | CD2 | LEU | 12 | 10.078 | 28.685 | 93.273 | 1.00 | 28.47 | AAGL |
| ATOM | 87 | C | LEU | 12 | 5.844 | 28.768 | 94.362 | 1.00 | 28.42 | AAGL |
| ATOM | 88 | O | LEU | 12 | 5.181 | 29.257 | 93.447 | 1.00 | 28.84 | AAGL |
| ATOM | 89 | N | LEU | 13 | 5.758 | 27.487 | 94.701 | 1.00 | 28.60 | AAGL |
| ATOM | 90 | CA | LEU | 13 | 4.879 | 26.590 | 93.963 | 1.00 | 30.83 | AAGL |
| ATOM | 91 | CB | LEU | 13 | 4.997 | 25.164 | 94.514 | 1.00 | 30.59 | AAGL |
| ATOM | 92 | CG | LEU | 13 | 6.443 | 24.657 | 94.640 | 1.00 | 29.90 | AAGL |
| ATOM | 93 | CD1 | LEU | 13 | 6.441 | 23.200 | 95.044 | 1.00 | 30.84 | AAGL |
| ATOM | 94 | CD2 | LEU | 13 | 7.179 | 24.821 | 93.315 | 1.00 | 31.95 | AAGL |
| ATOM | 95 | C | LEU | 13 | 3.430 | 27.062 | 93.967 | 1.00 | 31.99 | AAGL |
| ATOM | 96 | O | LEU | 13 | 2.703 | 26.844 | 93.001 | 1.00 | 33.62 | AAGL |
| ATOM | 97 | N | LEU | 14 | 3.008 | 27.725 | 95.038 | 1.00 | 33.18 | AAGL |
| ATOM | 98 | CA | LEU | 14 | 1.639 | 28.226 | 95.106 | 1.00 | 33.64 | AAGL |
| ATOM | 99 | CB | LEU | 14 | 1.289 | 28.683 | 96.523 | 1.00 | 34.87 | AAGL |
| ATOM | 100 | CG | LEU | 14 | 0.959 | 27.561 | 97.502 | 1.00 | 35.78 | AAGL |
| ATOM | 101 | CD1 | LEU | 14 | 0.492 | 28.145 | 98.828 | 1.00 | 36.41 | AAGL |
| ATOM | 102 | CD2 | LEU | 14 | −0.137 | 26.693 | 96.895 | 1.00 | 37.20 | AAGL |
| ATOM | 103 | C | LEU | 14 | 1.423 | 29.385 | 94.141 | 1.00 | 34.86 | AAGL |
| ATOM | 104 | O | LEU | 14 | 0.352 | 29.522 | 93.551 | 1.00 | 33.97 | AAGL |
| ATOM | 105 | N | LEU | 15 | 2.443 | 30.218 | 93.978 | 1.00 | 34.48 | AAGL |
| ATOM | 106 | CA | LEU | 15 | 2.344 | 31.359 | 93.080 | 1.00 | 35.10 | AAGL |
| ATOM | 107 | CB | LEU | 15 | 3.428 | 32.390 | 93.415 | 1.00 | 35.52 | AAGL |
| ATOM | 108 | CG | LEU | 15 | 3.232 | 33.227 | 94.696 | 1.00 | 37.21 | AAGL |
| ATOM | 109 | CD1 | LEU | 15 | 2.912 | 32.357 | 95.879 | 1.00 | 37.69 | AAGL |
| ATOM | 110 | CD2 | LEU | 15 | 4.496 | 34.018 | 94.975 | 1.00 | 35.91 | AAGL |
| ATOM | 111 | C | LEU | 15 | 2.458 | 30.904 | 91.624 | 1.00 | 35.48 | AAGL |
| ATOM | 112 | O | LEU | 15 | 1.647 | 31.306 | 90.782 | 1.00 | 35.67 | AAGL |
| ATOM | 113 | N | GLU | 16 | 3.449 | 30.065 | 91.329 | 1.00 | 35.68 | AAGL |
| ATOM | 114 | CA | GLU | 16 | 3.619 | 29.561 | 89.966 | 1.00 | 37.14 | AAGL |
| ATOM | 115 | CB | GLU | 16 | 4.747 | 28.527 | 89.890 | 1.00 | 35.01 | AAGL |
| ATOM | 116 | CG | GLU | 16 | 6.159 | 29.083 | 90.020 | 1.00 | 34.68 | AAGL |
| ATOM | 117 | CD | GLU | 16 | 7.214 | 27.993 | 89.905 | 1.00 | 35.45 | AAGL |
| ATOM | 118 | OE1 | GLU | 16 | 6.928 | 26.849 | 90.317 | 1.00 | 35.57 | AAGL |
| ATOM | 119 | OE2 | GLU | 16 | 8.336 | 28.271 | 89.419 | 1.00 | 35.12 | AAGL |
| ATOM | 120 | C | GLU | 16 | 2.317 | 28.913 | 89.527 | 1.00 | 39.70 | AAGL |
| ATOM | 121 | O | GLU | 16 | 1.846 | 29.139 | 88.411 | 1.00 | 40.81 | AAGL |
| ATOM | 122 | N | ASP | 17 | 1.727 | 28.112 | 90.411 | 1.00 | 41.41 | AAGL |
| ATOM | 123 | CA | ASP | 17 | 0.470 | 27.444 | 90.099 | 1.00 | 44.13 | AAGL |
| ATOM | 124 | CB | ASP | 17 | 0.029 | 26.557 | 91.262 | 1.00 | 44.94 | AAGL |
| ATOM | 125 | CG | ASP | 17 | 0.510 | 25.127 | 91.117 | 1.00 | 47.20 | AAGL |
| ATOM | 126 | OD1 | ASP | 17 | 0.423 | 24.359 | 92.103 | 1.00 | 47.97 | AAGL |
| ATOM | 127 | OD2 | ASP | 17 | 0.959 | 24.757 | 90.006 | 1.00 | 50.11 | AAGL |
| ATOM | 128 | C | ASP | 17 | −0.625 | 28.447 | 89.771 | 1.00 | 45.54 | AAGL |
| ATOM | 129 | O | ASP | 17 | −1.458 | 28.195 | 88.896 | 1.00 | 47.39 | AAGL |
| ATOM | 130 | N | GLU | 18 | −0.629 | 29.581 | 90.471 | 1.00 | 45.43 | AAGL |
| ATOM | 131 | CA | GLU | 18 | −1.625 | 30.617 | 90.234 | 1.00 | 47.08 | AAGL |

# Fig. 3 cont.

| ATOM | 132 | CB | GLU | 18 | -1.762 | 31.537 | 91.458 | 1.00 | 49.00 | AAGL |
| ATOM | 133 | CG | GLU | 18 | -2.526 | 30.900 | 92.622 | 1.00 | 52.65 | AAGL |
| ATOM | 134 | CD | GLU | 18 | -2.530 | 31.755 | 93.890 | 1.00 | 55.02 | AAGL |
| ATOM | 135 | OE1 | GLU | 18 | -3.112 | 31.305 | 94.911 | 1.00 | 55.65 | AAGL |
| ATOM | 136 | OE2 | GLU | 18 | -1.953 | 32.870 | 93.870 | 1.00 | 56.34 | AAGL |
| ATOM | 137 | C | GLU | 18 | -1.267 | 31.432 | 88.994 | 1.00 | 46.48 | AAGL |
| ATOM | 138 | O | GLU | 18 | -1.845 | 32.492 | 88.743 | 1.00 | 46.57 | AAGL |
| ATOM | 139 | N | GLY | 19 | -0.307 | 30.929 | 88.223 | 1.00 | 45.75 | AAGL |
| ATOM | 140 | CA | GLY | 19 | 0.091 | 31.609 | 87.006 | 1.00 | 45.53 | AAGL |
| ATOM | 141 | C | GLY | 19 | 1.245 | 32.588 | 87.113 | 1.00 | 45.29 | AAGL |
| ATOM | 142 | O | GLY | 19 | 1.636 | 33.185 | 86.113 | 1.00 | 44.87 | AAGL |
| ATOM | 143 | N | TYR | 20 | 1.802 | 32.758 | 88.309 | 1.00 | 44.55 | AAGL |
| ATOM | 144 | CA | TYR | 20 | 2.911 | 33.685 | 88.497 | 1.00 | 44.04 | AAGL |
| ATOM | 145 | CB | TYR | 20 | 3.098 | 33.987 | 89.985 | 1.00 | 46.33 | AAGL |
| ATOM | 146 | CG | TYR | 20 | 2.199 | 35.092 | 90.475 | 1.00 | 46.92 | AAGL |
| ATOM | 147 | CD1 | TYR | 20 | 1.174 | 34.837 | 91.384 | 1.00 | 47.92 | AAGL |
| ATOM | 148 | CE1 | TYR | 20 | 0.317 | 35.856 | 91.804 | 1.00 | 48.81 | AAGL |
| ATOM | 149 | CD2 | TYR | 20 | 2.351 | 36.388 | 89.995 | 1.00 | 48.25 | AAGL |
| ATOM | 150 | CE2 | TYR | 20 | 1.509 | 37.406 | 90.399 | 1.00 | 48.75 | AAGL |
| ATOM | 151 | CZ | TYR | 20 | 0.494 | 37.135 | 91.301 | 1.00 | 49.08 | AAGL |
| ATOM | 152 | OH | TYR | 20 | -0.350 | 38.146 | 91.676 | 1.00 | 50.05 | AAGL |
| ATOM | 153 | C | TYR | 20 | 4.243 | 33.232 | 87.916 | 1.00 | 42.70 | AAGL |
| ATOM | 154 | O | TYR | 20 | 4.541 | 32.043 | 87.857 | 1.00 | 41.19 | AAGL |
| ATOM | 155 | N | SER | 21 | 5.040 | 34.211 | 87.494 | 1.00 | 42.54 | AAGL |
| ATOM | 156 | CA | SER | 21 | 6.360 | 33.981 | 86.918 | 1.00 | 42.59 | AAGL |
| ATOM | 157 | CB | SER | 21 | 6.255 | 33.775 | 85.402 | 1.00 | 43.78 | AAGL |
| ATOM | 158 | OG | SER | 21 | 5.527 | 34.835 | 84.790 | 1.00 | 44.41 | AAGL |
| ATOM | 159 | C | SER | 21 | 7.191 | 35.224 | 87.221 | 1.00 | 41.81 | AAGL |
| ATOM | 160 | O | SER | 21 | 6.639 | 36.307 | 87.421 | 1.00 | 42.15 | AAGL |
| ATOM | 161 | N | TYR | 22 | 8.510 | 35.075 | 87.260 | 1.00 | 40.81 | AAGL |
| ATOM | 162 | CA | TYR | 22 | 9.382 | 36.205 | 87.558 | 1.00 | 40.63 | AAGL |
| ATOM | 163 | CB | TYR | 22 | 10.143 | 35.955 | 88.855 | 1.00 | 39.48 | AAGL |
| ATOM | 164 | CG | TYR | 22 | 9.248 | 35.579 | 90.010 | 1.00 | 37.92 | AAGL |
| ATOM | 165 | CD1 | TYR | 22 | 8.820 | 34.261 | 90.186 | 1.00 | 35.93 | AAGL |
| ATOM | 166 | CE1 | TYR | 22 | 7.987 | 33.913 | 91.246 | 1.00 | 35.62 | AAGL |
| ATOM | 167 | CD2 | TYR | 22 | 8.820 | 36.540 | 90.921 | 1.00 | 37.21 | AAGL |
| ATOM | 168 | CE2 | TYR | 22 | 7.982 | 36.204 | 91.982 | 1.00 | 35.75 | AAGL |
| ATOM | 169 | CZ | TYR | 22 | 7.574 | 34.897 | 92.140 | 1.00 | 36.41 | AAGL |
| ATOM | 170 | OH | TYR | 22 | 6.761 | 34.573 | 93.196 | 1.00 | 34.78 | AAGL |
| ATOM | 171 | C | TYR | 22 | 10.385 | 36.498 | 86.455 | 1.00 | 41.14 | AAGL |
| ATOM | 172 | O | TYR | 22 | 10.607 | 35.672 | 85.568 | 1.00 | 40.90 | AAGL |
| ATOM | 173 | N | LYS | 23 | 10.990 | 37.684 | 86.532 | 1.00 | 40.98 | AAGL |
| ATOM | 174 | CA | LYS | 23 | 11.987 | 38.131 | 85.565 | 1.00 | 41.42 | AAGL |
| ATOM | 175 | CB | LYS | 23 | 11.430 | 39.257 | 84.690 | 1.00 | 44.58 | AAGL |
| ATOM | 176 | CG | LYS | 23 | 10.779 | 38.781 | 83.398 | 1.00 | 49.11 | AAGL |
| ATOM | 177 | CD | LYS | 23 | 9.379 | 38.262 | 83.633 | 1.00 | 51.49 | AAGL |
| ATOM | 178 | CE | LYS | 23 | 8.453 | 39.401 | 84.042 | 1.00 | 52.49 | AAGL |
| ATOM | 179 | NZ | LYS | 23 | 8.461 | 40.487 | 83.021 | 1.00 | 51.35 | AAGL |
| ATOM | 180 | C | LYS | 23 | 13.248 | 38.634 | 86.243 | 1.00 | 40.33 | AAGL |
| ATOM | 181 | O | LYS | 23 | 13.184 | 39.363 | 87.241 | 1.00 | 39.11 | AAGL |
| ATOM | 182 | N | ASN | 24 | 14.396 | 38.246 | 85.693 | 1.00 | 38.79 | AAGL |
| ATOM | 183 | CA | ASN | 24 | 15.682 | 38.672 | 86.226 | 1.00 | 40.03 | AAGL |
| ATOM | 184 | CB | ASN | 24 | 16.807 | 37.935 | 85.509 | 1.00 | 42.29 | AAGL |
| ATOM | 185 | CG | ASN | 24 | 16.738 | 38.104 | 84.004 | 1.00 | 42.84 | AAGL |
| ATOM | 186 | OD1 | ASN | 24 | 16.732 | 39.224 | 83.497 | 1.00 | 43.55 | AAGL |
| ATOM | 187 | ND2 | ASN | 24 | 16.675 | 36.993 | 83.282 | 1.00 | 45.13 | AAGL |
| ATOM | 188 | C | ASN | 24 | 15.840 | 40.178 | 86.018 | 1.00 | 40.98 | AAGL |
| ATOM | 189 | O | ASN | 24 | 14.938 | 40.837 | 85.494 | 1.00 | 38.96 | AAGL |
| ATOM | 190 | N | LEU | 25 | 16.987 | 40.720 | 86.423 | 1.00 | 42.28 | AAGL |
| ATOM | 191 | CA | LEU | 25 | 17.246 | 42.149 | 86.283 | 1.00 | 44.49 | AAGL |
| ATOM | 192 | CB | LEU | 25 | 18.528 | 42.543 | 87.032 | 1.00 | 44.66 | AAGL |
| ATOM | 193 | CG | LEU | 25 | 18.549 | 42.643 | 88.563 | 1.00 | 45.79 | AAGL |
| ATOM | 194 | CD1 | LEU | 25 | 17.376 | 43.494 | 89.037 | 1.00 | 45.23 | AAGL |
| ATOM | 195 | CD2 | LEU | 25 | 18.493 | 41.252 | 89.189 | 1.00 | 46.13 | AAGL |
| ATOM | 196 | C | LEU | 25 | 17.345 | 42.614 | 84.824 | 1.00 | 45.76 | AAGL |
| ATOM | 197 | O | LEU | 25 | 17.454 | 43.814 | 84.562 | 1.00 | 46.23 | AAGL |

# Fig. 3 cont.

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ATOM    198   N    ASN   26      17.311   41.675   83.880   1.00  46.41          AAGL
ATOM    199   CA   ASN   26      17.365   42.021   82.455   1.00  47.05          AAGL
ATOM    200   CB   ASN   26      18.288   41.066   81.676   1.00  47.42          AAGL
ATOM    201   CG   ASN   26      19.747   41.198   82.074   1.00  49.18          AAGL
ATOM    202   OD1  ASN   26      20.207   42.276   82.459   1.00  49.93          AAGL
ATOM    203   ND2  ASN   26      20.492   40.100   81.961   1.00  49.97          AAGL
ATOM    204   C    ASN   26      15.966   41.947   81.848   1.00  47.00          AAGL
ATOM    205   O    ASN   26      15.796   42.082   80.634   1.00  47.34          AAGL
ATOM    206   N    GLY   27      14.961   41.712   82.684   1.00  45.83          AAGL
ATOM    207   CA   GLY   27      13.602   41.628   82.176   1.00  45.48          AAGL
ATOM    208   C    GLY   27      13.343   40.327   81.436   1.00  45.43          AAGL
ATOM    209   O    GLY   27      12.388   40.225   80.669   1.00  46.84          AAGL
ATOM    210   N    GLN   28      14.198   39.332   81.648   1.00  45.03          AAGL
ATOM    211   CA   GLN   28      14.023   38.037   81.002   1.00  44.89          AAGL
ATOM    212   CB   GLN   28      15.385   37.428   80.633   1.00  46.09          AAGL
ATOM    213   CG   GLN   28      16.346   38.371   79.909   1.00  48.72          AAGL
ATOM    214   CD   GLN   28      17.649   37.684   79.531   1.00  49.91          AAGL
ATOM    215   OE1  GLN   28      17.674   36.802   78.668   1.00  51.23          AAGL
ATOM    216   NE2  GLN   28      18.740   38.075   80.187   1.00  51.05          AAGL
ATOM    217   C    GLN   28      13.312   37.093   81.980   1.00  43.57          AAGL
ATOM    218   O    GLN   28      13.800   36.871   83.088   1.00  40.72          AAGL
ATOM    219   N    THR   29      12.166   36.542   81.580   1.00  42.64          AAGL
ATOM    220   CA   THR   29      11.441   35.610   82.445   1.00  42.01          AAGL
ATOM    221   CB   THR   29      10.201   35.022   81.746   1.00  42.12          AAGL
ATOM    222   OG1  THR   29       9.191   36.030   81.626   1.00  42.02          AAGL
ATOM    223   CG2  THR   29       9.639   33.857   82.552   1.00  41.97          AAGL
ATOM    224   C    THR   29      12.393   34.472   82.787   1.00  41.90          AAGL
ATOM    225   O    THR   29      13.233   34.095   81.966   1.00  41.33          AAGL
ATOM    226   N    GLN   30      12.261   33.909   83.984   1.00  40.58          AAGL
ATOM    227   CA   GLN   30      13.158   32.835   84.392   1.00  39.49          AAGL
ATOM    228   CB   GLN   30      14.585   33.383   84.396   1.00  40.50          AAGL
ATOM    229   CG   GLN   30      15.604   32.528   85.100   1.00  43.69          AAGL
ATOM    230   CD   GLN   30      17.014   33.031   84.892   1.00  46.36          AAGL
ATOM    231   OE1  GLN   30      17.325   34.200   85.159   1.00  45.16          AAGL
ATOM    232   NE2  GLN   30      17.888   32.145   84.409   1.00  47.79          AAGL
ATOM    233   C    GLN   30      12.790   32.268   85.763   1.00  38.44          AAGL
ATOM    234   O    GLN   30      12.368   33.004   86.656   1.00  38.87          AAGL
ATOM    235   N    ALA   31      12.946   30.958   85.929   1.00  36.80          AAGL
ATOM    236   CA   ALA   31      12.617   30.314   87.202   1.00  34.49          AAGL
ATOM    237   CB   ALA   31      13.079   28.855   87.186   1.00  34.38          AAGL
ATOM    238   C    ALA   31      13.261   31.059   88.371   1.00  32.91          AAGL
ATOM    239   O    ALA   31      14.474   31.278   88.392   1.00  32.07          AAGL
ATOM    240   N    LEU   32      12.441   31.432   89.352   1.00  33.31          AAGL
ATOM    241   CA   LEU   32      12.914   32.180   90.522   1.00  29.54          AAGL
ATOM    242   CB   LEU   32      11.809   32.294   91.574   1.00  28.70          AAGL
ATOM    243   CG   LEU   32      12.229   33.100   92.815   1.00  26.84          AAGL
ATOM    244   CD1  LEU   32      12.430   34.545   92.422   1.00  26.55          AAGL
ATOM    245   CD2  LEU   32      11.173   32.985   93.916   1.00  26.84          AAGL
ATOM    246   C    LEU   32      14.160   31.618   91.192   1.00  30.30          AAGL
ATOM    247   O    LEU   32      15.068   32.375   91.545   1.00  29.24          AAGL
ATOM    248   N    GLU   33      14.205   30.304   91.387   1.00  29.20          AAGL
ATOM    249   CA   GLU   33      15.360   29.698   92.036   1.00  29.33          AAGL
ATOM    250   CB   GLU   33      15.164   28.184   92.223   1.00  30.11          AAGL
ATOM    251   CG   GLU   33      15.225   27.380   90.934   1.00  32.96          AAGL
ATOM    252   CD   GLU   33      13.872   27.167   90.294   1.00  32.82          AAGL
ATOM    253   OE1  GLU   33      12.979   28.030   90.451   1.00  32.32          AAGL
ATOM    254   OE2  GLU   33      13.706   26.126   89.609   1.00  34.46          AAGL
ATOM    255   C    GLU   33      16.641   29.949   91.242   1.00  30.20          AAGL
ATOM    256   O    GLU   33      17.708   30.125   91.828   1.00  30.32          AAGL
ATOM    257   N    THR   34      16.544   29.967   89.912   1.00  31.16          AAGL
ATOM    258   CA   THR   34      17.734   30.197   89.102   1.00  32.16          AAGL
ATOM    259   CB   THR   34      17.545   29.703   87.636   1.00  34.39          AAGL
ATOM    260   OG1  THR   34      16.690   30.598   86.916   1.00  39.01          AAGL
ATOM    261   CG2  THR   34      16.915   28.315   87.628   1.00  33.29          AAGL
ATOM    262   C    THR   34      18.100   31.677   89.120   1.00  30.19          AAGL
ATOM    263   O    THR   34      19.269   32.027   89.031   1.00  32.36          AAGL
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# Fig. 3 cont.

| ATOM | 264 | N | ILE | 35 | 17.101 | 32.542 | 89.254 | 1.00 29.48 | AAGL |
|------|-----|-----|-----|-----|--------|--------|---------|------------|------|
| ATOM | 265 | CA | ILE | 35 | 17.343 | 33.982 | 89.318 | 1.00 29.20 | AAGL |
| ATOM | 266 | CB | ILE | 35 | 16.030 | 34.783 | 89.364 | 1.00 29.36 | AAGL |
| ATOM | 267 | CG2 | ILE | 35 | 16.329 | 36.253 | 89.647 | 1.00 32.47 | AAGL |
| ATOM | 268 | CG1 | ILE | 35 | 15.265 | 34.620 | 88.052 | 1.00 30.39 | AAGL |
| ATOM | 269 | CD1 | ILE | 35 | 13.998 | 35.456 | 87.981 | 1.00 32.09 | AAGL |
| ATOM | 270 | C | ILE | 35 | 18.103 | 34.276 | 90.605 | 1.00 29.48 | AAGL |
| ATOM | 271 | O | ILE | 35 | 19.039 | 35.068 | 90.627 | 1.00 28.30 | AAGL |
| ATOM | 272 | N | LEU | 36 | 17.676 | 33.631 | 91.684 | 1.00 28.93 | AAGL |
| ATOM | 273 | CA | LEU | 36 | 18.297 | 33.809 | 92.989 | 1.00 27.40 | AAGL |
| ATOM | 274 | CB | LEU | 36 | 17.420 | 33.142 | 94.050 | 1.00 29.01 | AAGL |
| ATOM | 275 | CG | LEU | 36 | 16.067 | 33.824 | 94.220 | 1.00 29.41 | AAGL |
| ATOM | 276 | CD1 | LEU | 36 | 15.139 | 32.993 | 95.105 | 1.00 32.23 | AAGL |
| ATOM | 277 | CD2 | LEU | 36 | 16.318 | 35.198 | 94.831 | 1.00 29.88 | AAGL |
| ATOM | 278 | C | LEU | 36 | 19.693 | 33.220 | 93.036 | 1.00 26.84 | AAGL |
| ATOM | 279 | O | LEU | 36 | 20.630 | 33.840 | 93.542 | 1.00 26.88 | AAGL |
| ATOM | 280 | N | ALA | 37 | 19.829 | 32.005 | 92.515 | 1.00 28.77 | AAGL |
| ATOM | 281 | CA | ALA | 37 | 21.118 | 31.325 | 92.509 | 1.00 30.25 | AAGL |
| ATOM | 282 | CB | ALA | 37 | 20.988 | 29.971 | 91.805 | 1.00 29.94 | AAGL |
| ATOM | 283 | C | ALA | 37 | 22.185 | 32.180 | 91.827 | 1.00 29.84 | AAGL |
| ATOM | 284 | O | ALA | 37 | 23.274 | 32.373 | 92.365 | 1.00 30.61 | AAGL |
| ATOM | 285 | N | ASP | 38 | 21.856 | 32.706 | 90.652 | 1.00 30.68 | AAGL |
| ATOM | 286 | CA | ASP | 38 | 22.798 | 33.524 | 89.894 | 1.00 31.88 | AAGL |
| ATOM | 287 | CB | ASP | 38 | 22.240 | 33.843 | 88.508 | 1.00 32.57 | AAGL |
| ATOM | 288 | CG | ASP | 38 | 22.007 | 32.603 | 87.673 | 1.00 36.25 | AAGL |
| ATOM | 289 | OD1 | ASP | 38 | 22.749 | 31.610 | 87.859 | 1.00 36.97 | AAGL |
| ATOM | 290 | OD2 | ASP | 38 | 21.085 | 32.621 | 86.830 | 1.00 37.38 | AAGL |
| ATOM | 291 | C | ASP | 38 | 23.127 | 34.824 | 90.601 | 1.00 31.89 | AAGL |
| ATOM | 292 | O | ASP | 38 | 24.174 | 35.423 | 90.353 | 1.00 33.41 | AAGL |
| ATOM | 293 | N | ALA | 39 | 22.226 | 35.265 | 91.476 | 1.00 31.50 | AAGL |
| ATOM | 294 | CA | ALA | 39 | 22.433 | 36.503 | 92.207 | 1.00 29.58 | AAGL |
| ATOM | 295 | CB | ALA | 39 | 21.088 | 37.099 | 92.626 | 1.00 29.62 | AAGL |
| ATOM | 296 | C | ALA | 39 | 23.319 | 36.300 | 93.423 | 1.00 29.11 | AAGL |
| ATOM | 297 | O | ALA | 39 | 23.739 | 37.268 | 94.053 | 1.00 28.08 | AAGL |
| ATOM | 298 | N | GLY | 40 | 23.603 | 35.047 | 93.769 | 1.00 28.38 | AAGL |
| ATOM | 299 | CA | GLY | 40 | 24.462 | 34.804 | 94.915 | 1.00 28.68 | AAGL |
| ATOM | 300 | C | GLY | 40 | 23.804 | 34.079 | 96.077 | 1.00 27.30 | AAGL |
| ATOM | 301 | O | GLY | 40 | 24.489 | 33.628 | 96.994 | 1.00 28.21 | AAGL |
| ATOM | 302 | N | ILE | 41 | 22.480 | 33.973 | 96.046 | 1.00 27.82 | AAGL |
| ATOM | 303 | CA | ILE | 41 | 21.754 | 33.271 | 97.105 | 1.00 28.31 | AAGL |
| ATOM | 304 | CB | ILE | 41 | 20.231 | 33.267 | 96.841 | 1.00 28.86 | AAGL |
| ATOM | 305 | CG2 | ILE | 41 | 19.502 | 32.678 | 98.047 | 1.00 26.11 | AAGL |
| ATOM | 306 | CG1 | ILE | 41 | 19.741 | 34.680 | 96.490 | 1.00 32.71 | AAGL |
| ATOM | 307 | CD1 | ILE | 41 | 20.041 | 35.739 | 97.526 | 1.00 34.86 | AAGL |
| ATOM | 308 | C | ILE | 41 | 22.262 | 31.830 | 97.055 | 1.00 29.05 | AAGL |
| ATOM | 309 | O | ILE | 41 | 22.275 | 31.223 | 95.982 | 1.00 28.58 | AAGL |
| ATOM | 310 | N | ASN | 42 | 22.694 | 31.283 | 98.192 | 1.00 27.24 | AAGL |
| ATOM | 311 | CA | ASN | 42 | 23.209 | 29.921 | 98.192 | 1.00 27.38 | AAGL |
| ATOM | 312 | CB | ASN | 42 | 24.715 | 29.897 | 98.547 | 1.00 26.67 | AAGL |
| ATOM | 313 | CG | ASN | 42 | 25.014 | 30.267 | 99.999 | 1.00 29.27 | AAGL |
| ATOM | 314 | OD1 | ASN | 42 | 26.177 | 30.238 | 100.422 | 1.00 30.70 | AAGL |
| ATOM | 315 | ND2 | ASN | 42 | 23.984 | 30.620 | 100.767 | 1.00 28.35 | AAGL |
| ATOM | 316 | C | ASN | 42 | 22.449 | 28.945 | 99.077 | 1.00 27.09 | AAGL |
| ATOM | 317 | O | ASN | 42 | 22.873 | 27.801 | 99.244 | 1.00 25.65 | AAGL |
| ATOM | 318 | N | SER | 43 | 21.324 | 29.390 | 99.633 | 1.00 25.87 | AAGL |
| ATOM | 319 | CA | SER | 43 | 20.525 | 28.520 | 100.481 | 1.00 25.56 | AAGL |
| ATOM | 320 | CB | SER | 43 | 21.049 | 28.551 | 101.913 | 1.00 26.01 | AAGL |
| ATOM | 321 | OG | SER | 43 | 20.497 | 27.483 | 102.665 | 1.00 25.97 | AAGL |
| ATOM | 322 | C | SER | 43 | 19.051 | 28.914 | 100.462 | 1.00 25.21 | AAGL |
| ATOM | 323 | O | SER | 43 | 18.714 | 30.096 | 100.411 | 1.00 22.67 | AAGL |
| ATOM | 324 | N | ILE | 44 | 18.177 | 27.910 | 100.494 | 1.00 24.04 | AAGL |
| ATOM | 325 | CA | ILE | 44 | 16.737 | 28.146 | 100.475 | 1.00 23.25 | AAGL |
| ATOM | 326 | CB | ILE | 44 | 16.105 | 27.603 | 99.166 | 1.00 25.17 | AAGL |
| ATOM | 327 | CG2 | ILE | 44 | 14.599 | 27.796 | 99.185 | 1.00 23.06 | AAGL |
| ATOM | 328 | CG1 | ILE | 44 | 16.698 | 28.333 | 97.953 | 1.00 25.29 | AAGL |
| ATOM | 329 | CD1 | ILE | 44 | 16.327 | 29.795 | 97.867 | 1.00 26.67 | AAGL |

# Fig. 3 cont.

| ATOM | 330 | C | ILE | 44 | 16.057 | 27.481 | 101.677 | 1.00 | 23.88 | AAGL |
|------|-----|-----|-----|----|--------|--------|---------|------|-------|------|
| ATOM | 331 | O | ILE | 44 | 16.273 | 26.305 | 101.953 | 1.00 | 22.19 | AAGL |
| ATOM | 332 | N | ARG | 45 | 15.244 | 28.262 | 102.384 | 1.00 | 21.15 | AAGL |
| ATOM | 333 | CA | ARG | 45 | 14.512 | 27.796 | 103.558 | 1.00 | 20.84 | AAGL |
| ATOM | 334 | CB | ARG | 45 | 14.497 | 28.905 | 104.607 | 1.00 | 19.60 | AAGL |
| ATOM | 335 | CG | ARG | 45 | 13.815 | 28.594 | 105.927 | 1.00 | 22.30 | AAGL |
| ATOM | 336 | CD | ARG | 45 | 13.941 | 29.840 | 106.803 | 1.00 | 22.44 | AAGL |
| ATOM | 337 | NE | ARG | 45 | 13.442 | 29.713 | 108.172 | 1.00 | 21.57 | AAGL |
| ATOM | 338 | CZ | ARG | 45 | 12.253 | 30.147 | 108.580 | 1.00 | 21.21 | AAGL |
| ATOM | 339 | NH1 | ARG | 45 | 11.420 | 30.721 | 107.726 | 1.00 | 19.38 | AAGL |
| ATOM | 340 | NH2 | ARG | 45 | 11.924 | 30.071 | 109.864 | 1.00 | 18.87 | AAGL |
| ATOM | 341 | C | ARG | 45 | 13.091 | 27.456 | 103.120 | 1.00 | 18.60 | AAGL |
| ATOM | 342 | O | ARG | 45 | 12.471 | 28.214 | 102.376 | 1.00 | 19.88 | AAGL |
| ATOM | 343 | N | GLN | 46 | 12.582 | 26.314 | 103.574 | 1.00 | 19.69 | AAGL |
| ATOM | 344 | CA | GLN | 46 | 11.235 | 25.881 | 103.212 | 1.00 | 18.26 | AAGL |
| ATOM | 345 | CB | GLN | 46 | 11.311 | 24.701 | 102.234 | 1.00 | 19.90 | AAGL |
| ATOM | 346 | CG | GLN | 46 | 12.070 | 25.027 | 100.949 | 1.00 | 19.68 | AAGL |
| ATOM | 347 | CD | GLN | 46 | 12.093 | 23.880 | 99.946 | 1.00 | 23.43 | AAGL |
| ATOM | 348 | OE1 | GLN | 46 | 12.705 | 23.992 | 98.882 | 1.00 | 26.77 | AAGL |
| ATOM | 349 | NE2 | GLN | 46 | 11.429 | 22.777 | 100.278 | 1.00 | 21.73 | AAGL |
| ATOM | 350 | C | GLN | 46 | 10.432 | 25.467 | 104.445 | 1.00 | 17.71 | AAGL |
| ATOM | 351 | O | GLN | 46 | 10.896 | 24.649 | 105.238 | 1.00 | 18.22 | AAGL |
| ATOM | 352 | N | ARG | 47 | 9.233 | 26.023 | 104.601 | 1.00 | 18.28 | AAGL |
| ATOM | 353 | CA | ARG | 47 | 8.409 | 25.670 | 105.751 | 1.00 | 18.38 | AAGL |
| ATOM | 354 | CB | ARG | 47 | 7.414 | 26.792 | 106.095 | 1.00 | 18.50 | AAGL |
| ATOM | 355 | CG | ARG | 47 | 6.542 | 27.319 | 104.954 | 1.00 | 21.41 | AAGL |
| ATOM | 356 | CD | ARG | 47 | 5.455 | 28.254 | 105.503 | 1.00 | 20.07 | AAGL |
| ATOM | 357 | NE | ARG | 47 | 4.735 | 28.978 | 104.453 | 1.00 | 18.68 | AAGL |
| ATOM | 358 | CZ | ARG | 47 | 5.228 | 30.016 | 103.783 | 1.00 | 19.34 | AAGL |
| ATOM | 359 | NH1 | ARG | 47 | 6.448 | 30.472 | 104.054 | 1.00 | 20.84 | AAGL |
| ATOM | 360 | NH2 | ARG | 47 | 4.513 | 30.582 | 102.819 | 1.00 | 19.53 | AAGL |
| ATOM | 361 | C | ARG | 47 | 7.677 | 24.365 | 105.472 | 1.00 | 18.74 | AAGL |
| ATOM | 362 | O | ARG | 47 | 7.101 | 24.183 | 104.403 | 1.00 | 18.19 | AAGL |
| ATOM | 363 | N | VAL | 48 | 7.710 | 23.458 | 106.445 | 1.00 | 19.24 | AAGL |
| ATOM . | 364 | CA | VAL | 48 | 7.074 | 22.155 | 106.301 | 1.00 | 20.17 | AAGL |
| ATOM | 365 | CB | VAL | 48 | 8.109 | 21.023 | 106.490 | 1.00 | 20.89 | AAGL |
| ATOM | 366 | CG1 | VAL | 48 | 7.488 | 19.677 | 106.130 | 1.00 | 20.76 | AAGL |
| ATOM | 367 | CG2 | VAL | 48 | 9.350 | 21.301 | 105.644 | 1.00 | 21.80 | AAGL |
| ATOM | 368 | C | VAL | 48 | 5.947 | 21.932 | 107.311 | 1.00 | 20.72 | AAGL |
| ATOM | 369 | O | VAL | 48 | 6.166 | 22.027 | 108.517 | 1.00 | 19.48 | AAGL |
| ATOM | 370 | N | TRP | 49 | 4.748 | 21.647 | 106.805 | 1.00 | 18.93 | AAGL |
| ATOM | 371 | CA | TRP | 49 | 3.590 | 21.371 | 107.646 | 1.00 | 19.06 | AAGL |
| ATOM | 372 | CB | TRP | 49 | 2.382 | 22.168 | 107.167 | 1.00 | 19.85 | AAGL |
| ATOM | 373 | CG | TRP | 49 | 2.525 | 23.645 | 107.414 | 1.00 | 19.05 | AAGL |
| ATOM | 374 | CD2 | TRP | 49 | 1.608 | 24.673 | 107.024 | 1.00 | 18.82 | AAGL |
| ATOM | 375 | CE2 | TRP | 49 | 2.125 | 25.897 | 107.504 | 1.00 | 19.73 | AAGL |
| ATOM | 376 | CE3 | TRP | 49 | 0.396 | 24.678 | 106.316 | 1.00 | 20.02 | AAGL |
| ATOM | 377 | CD1 | TRP | 49 | 3.535 | 24.271 | 108.090 | 1.00 | 17.67 | AAGL |
| ATOM | 378 | NE1 | TRP | 49 | 3.300 | 25.620 | 108.149 | 1.00 | 18.03 | AAGL |
| ATOM | 379 | CZ2 | TRP | 49 | 1.475 | 27.117 | 107.301 | 1.00 | 20.25 | AAGL |
| ATOM | 380 | CZ3 | TRP | 49 | −0.253 | 25.899 | 106.112 | 1.00 | 22.82 | AAGL |
| ATOM | 381 | CH2 | TRP | 49 | 0.291 | 27.100 | 106.606 | 1.00 | 22.06 | AAGL |
| ATOM | 382 | C | TRP | 49 | 3.306 | 19.873 | 107.587 | 1.00 | 19.52 | AAGL |
| ATOM | 383 | O | TRP | 49 | 3.553 | 19.231 | 106.563 | 1.00 | 19.96 | AAGL |
| ATOM | 384 | N | VAL | 50 | 2.778 | 19.322 | 108.677 | 1.00 | 18.80 | AAGL |
| ATOM | 385 | CA | VAL | 50 | 2.522 | 17.886 | 108.756 | 1.00 | 20.11 | AAGL |
| ATOM | 386 | CB | VAL | 50 | 2.398 | 17.443 | 110.231 | 1.00 | 18.82 | AAGL |
| ATOM | 387 | CG1 | VAL | 50 | 2.120 | 15.954 | 110.316 | 1.00 | 21.34 | AAGL |
| ATOM | 388 | CG2 | VAL | 50 | 3.695 | 17.768 | 110.966 | 1.00 | 21.13 | AAGL |
| ATOM | 389 | C | VAL | 50 | 1.340 | 17.362 | 107.947 | 1.00 | 22.22 | AAGL |
| ATOM | 390 | O | VAL | 50 | 1.538 | 16.629 | 106.973 | 1.00 | 23.75 | AAGL |
| ATOM | 391 | N | ASN | 51 | 0.119 | 17.721 | 108.329 | 1.00 | 22.74 | AAGL |
| ATOM | 392 | CA | ASN | 51 | −1.044 | 17.251 | 107.585 | 1.00 | 25.51 | AAGL |
| ATOM | 393 | CB | ASN | 51 | −1.765 | 16.133 | 108.354 | 1.00 | 26.96 | AAGL |
| ATOM | 394 | CG | ASN | 51 | −0.879 | 14.932 | 108.619 | 0.50 | 27.07 | AAGL |
| ATOM | 395 | OD1 | ASN | 51 | −0.265 | 14.387 | 107.707 | 0.50 | 29.27 | AAGL |

# Fig. 3 cont.

| ATOM | 396 | ND2 | ASN | 51 | -0.821 | 14.505 | 109.878 | 0.50 | 28.87 | AAGL |
|------|-----|-----|-----|----|--------|--------|---------|------|-------|------|
| ATOM | 397 | C | ASN | 51 | -2.055 | 18.350 | 107.238 | 1.00 | 26.72 | AAGL |
| ATOM | 398 | O | ASN | 51 | -3.204 | 18.305 | 107.668 | 1.00 | 27.90 | AAGL |
| ATOM | 399 | N | PRO | 52 | -1.638 | 19.358 | 106.459 | 1.00 | 26.25 | AAGL |
| ATOM | 400 | CD | PRO | 52 | -0.337 | 19.594 | 105.814 | 1.00 | 25.34 | AAGL |
| ATOM | 401 | CA | PRO | 52 | -2.599 | 20.410 | 106.113 | 1.00 | 26.62 | AAGL |
| ATOM | 402 | CB | PRO | 52 | -1.735 | 21.431 | 105.389 | 1.00 | 25.68 | AAGL |
| ATOM | 403 | CG | PRO | 52 | -0.697 | 20.582 | 104.735 | 1.00 | 25.47 | AAGL |
| ATOM | 404 | C | PRO | 52 | -3.690 | 19.816 | 105.215 | 1.00 | 28.63 | AAGL |
| ATOM | 405 | O | PRO | 52 | -3.391 | 19.112 | 104.254 | 1.00 | 27.01 | AAGL |
| ATOM | 406 | N | SER | 53 | -4.949 | 20.086 | 105.543 | 1.00 | 29.82 | AAGL |
| ATOM | 407 | CA | SER | 53 | -6.062 | 19.554 | 104.760 | 1.00 | 33.18 | AAGL |
| ATOM | 408 | CB | SER | 53 | -7.394 | 20.100 | 105.281 | 1.00 | 35.65 | AAGL |
| ATOM | 409 | OG | SER | 53 | -7.728 | 19.496 | 106.515 | 1.00 | 38.67 | AAGL |
| ATOM | 410 | C | SER | 53 | -5.948 | 19.859 | 103.274 | 1.00 | 32.30 | AAGL |
| ATOM | 411 | O | SER | 53 | -6.284 | 19.019 | 102.434 | 1.00 | 32.67 | AAGL |
| ATOM | 412 | N | ASP | 54 | -5.469 | 21.053 | 102.949 | 1.00 | 31.58 | AAGL |
| ATOM | 413 | CA | ASP | 54 | -5.343 | 21.444 | 101.555 | 1.00 | 31.37 | AAGL |
| ATOM | 414 | CB | ASP | 54 | -5.736 | 22.922 | 101.389 | 1.00 | 33.51 | AAGL |
| ATOM | 415 | CG | ASP | 54 | -4.616 | 23.878 | 101.754 | 1.00 | 35.96 | AAGL |
| ATOM | 416 | OD1 | ASP | 54 | -3.796 | 23.537 | 102.630 | 1.00 | 35.79 | AAGL |
| ATOM | 417 | OD2 | ASP | 54 | -4.569 | 24.986 | 101.166 | 1.00 | 38.48 | AAGL |
| ATOM | 418 | C | ASP | 54 | -3.974 | 21.164 | 100.937 | 1.00 | 30.51 | AAGL |
| ATOM | 419 | O | ASP | 54 | -3.715 | 21.572 | 99.812 | 1.00 | 30.89 | AAGL |
| ATOM | 420 | N | GLY | 55 | -3.110 | 20.460 | 101.670 | 1.00 | 31.08 | AAGL |
| ATOM | 421 | CA | GLY | 55 | -1.790 | 20.102 | 101.161 | 1.00 | 29.00 | AAGL |
| ATOM | 422 | C | GLY | 55 | -0.684 | 21.149 | 101.119 | 1.00 | 28.85 | AAGL |
| ATOM | 423 | O | GLY | 55 | 0.475 | 20.829 | 100.834 | 1.00 | 27.57 | AAGL |
| ATOM | 424 | N | SER | 56 | -1.028 | 22.399 | 101.398 | 1.00 | 29.06 | AAGL |
| ATOM | 425 | CA | SER | 56 | -0.036 | 23.468 | 101.362 | 1.00 | 29.25 | AAGL |
| ATOM | 426 | CB | SER | 56 | -0.685 | 24.799 | 101.747 | 1.00 | 33.01 | AAGL |
| ATOM | 427 | OG | SER | 56 | -1.603 | 25.222 | 100.746 | 1.00 | 35.28 | AAGL |
| ATOM | 428 | C | SER | 56 | 1.163 | 23.211 | 102.266 | 1.00 | 27.16 | AAGL |
| ATOM | 429 | O | SER | 56 | 1.013 | 22.944 | 103.462 | 1.00 | 26.75 | AAGL |
| ATOM | 430 | N | TYR | 57 | 2.350 | 23.282 | 101.673 | 1.00 | 24.25 | AAGL |
| ATOM | 431 | CA | TYR | 57 | 3.611 | 23.102 | 102.379 | 1.00 | 23.39 | AAGL |
| ATOM | 432 | CB | TYR | 57 | 3.773 | 24.192 | 103.455 | 1.00 | 21.44 | AAGL |
| ATOM | 433 | CG | TYR | 57 | 3.411 | 25.586 | 102.983 | 1.00 | 18.93 | AAGL |
| ATOM | 434 | CD1 | TYR | 57 | 4.090 | 26.183 | 101.927 | 1.00 | 20.85 | AAGL |
| ATOM | 435 | CE1 | TYR | 57 | 3.733 | 27.448 | 101.457 | 1.00 | 20.55 | AAGL |
| ATOM | 436 | CD2 | TYR | 57 | 2.363 | 26.291 | 103.575 | 1.00 | 20.42 | AAGL |
| ATOM | 437 | CE2 | TYR | 57 | 1.992 | 27.555 | 103.119 | 1.00 | 23.25 | AAGL |
| ATOM | 438 | CZ | TYR | 57 | 2.687 | 28.130 | 102.049 | 1.00 | 22.03 | AAGL |
| ATOM | 439 | OH | TYR | 57 | 2.323 | 29.367 | 101.572 | 1.00 | 24.57 | AAGL |
| ATOM | 440 | C | TYR | 57 | 3.809 | 21.736 | 103.024 | 1.00 | 24.63 | AAGL |
| ATOM | 441 | O | TYR | 57 | 4.583 | 21.619 | 103.972 | 1.00 | 22.67 | AAGL |
| ATOM | 442 | N | ASP | 58 | 3.121 | 20.701 | 102.540 | 1.00 | 25.81 | AAGL |
| ATOM | 443 | CA | ASP | 58 | 3.319 | 19.376 | 103.128 | 1.00 | 27.04 | AAGL |
| ATOM | 444 | CB | ASP | 58 | 2.084 | 18.473 | 102.946 | 1.00 | 27.80 | AAGL |
| ATOM | 445 | CG | ASP | 58 | 1.763 | 18.160 | 101.491 | 1.00 | 32.21 | AAGL |
| ATOM | 446 | OD1 | ASP | 58 | 2.652 | 18.279 | 100.623 | 1.00 | 30.26 | AAGL |
| ATOM | 447 | OD2 | ASP | 58 | 0.597 | 17.768 | 101.228 | 1.00 | 32.38 | AAGL |
| ATOM | 448 | C | ASP | 58 | 4.574 | 18.724 | 102.542 | 1.00 | 28.05 | AAGL |
| ATOM | 449 | O | ASP | 58 | 5.320 | 19.367 | 101.793 | 1.00 | 27.53 | AAGL |
| ATOM | 450 | N | LEU | 59 | 4.820 | 17.462 | 102.883 | 1.00 | 26.92 | AAGL |
| ATOM | 451 | CA | LEU | 59 | 6.018 | 16.786 | 102.403 | 1.00 | 28.31 | AAGL |
| ATOM | 452 | CB | LEU | 59 | 6.116 | 15.377 | 103.001 | 1.00 | 30.14 | AAGL |
| ATOM | 453 | CG | LEU | 59 | 7.435 | 14.620 | 102.784 | 1.00 | 29.84 | AAGL |
| ATOM | 454 | CD1 | LEU | 59 | 8.609 | 15.430 | 103.323 | 1.00 | 31.61 | AAGL |
| ATOM | 455 | CD2 | LEU | 59 | 7.355 | 13.265 | 103.479 | 1.00 | 31.80 | AAGL |
| ATOM | 456 | C | LEU | 59 | 6.145 | 16.714 | 100.885 | 1.00 | 26.89 | AAGL |
| ATOM | 457 | O | LEU | 59 | 7.220 | 16.952 | 100.342 | 1.00 | 24.30 | AAGL |
| ATOM | 458 | N | ASP | 60 | 5.061 | 16.401 | 100.188 | 1.00 | 28.43 | AAGL |
| ATOM | 459 | CA | ASP | 60 | 5.145 | 16.315 | 98.736 | 1.00 | 29.43 | AAGL |
| ATOM | 460 | CB | ASP | 60 | 3.850 | 15.740 | 98.149 | 1.00 | 32.44 | AAGL |
| ATOM | 461 | CG | ASP | 60 | 3.557 | 14.332 | 98.651 | 1.00 | 37.53 | AAGL |

# Fig. 3 cont.

| ATOM | 462 | OD1 | ASP | 60 | 4.518 | 13.547 | 98.833 | 1.00 | 40.66 | AAGL |
|------|-----|-----|-----|-----|-------|--------|--------|------|-------|------|
| ATOM | 463 | OD2 | ASP | 60 | 2.365 | 14.000 | 98.858 | 1.00 | 42.65 | AAGL |
| ATOM | 464 | C | ASP | 60 | 5.439 | 17.689 | 98.137 | 1.00 | 30.40 | AAGL |
| ATOM | 465 | O | ASP | 60 | 6.266 | 17.816 | 97.237 | 1.00 | 28.80 | AAGL |
| ATOM | 466 | N | TYR | 61 | 4.761 | 18.710 | 98.651 | 1.00 | 28.48 | AAGL |
| ATOM | 467 | CA | TYR | 61 | 4.944 | 20.088 | 98.203 | 1.00 | 25.60 | AAGL |
| ATOM | 468 | CB | TYR | 61 | 4.100 | 21.031 | 99.080 | 1.00 | 25.21 | AAGL |
| ATOM | 469 | CG | TYR | 61 | 4.182 | 22.508 | 98.723 | 1.00 | 25.14 | AAGL |
| ATOM | 470 | CD1 | TYR | 61 | 5.283 | 23.286 | 99.095 | 1.00 | 23.80 | AAGL |
| ATOM | 471 | CE1 | TYR | 61 | 5.360 | 24.639 | 98.759 | 1.00 | 24.64 | AAGL |
| ATOM | 472 | CD2 | TYR | 61 | 3.154 | 23.125 | 98.006 | 1.00 | 25.32 | AAGL |
| ATOM | 473 | CE2 | TYR | 61 | 3.220 | 24.481 | 97.664 | 1.00 | 26.31 | AAGL |
| ATOM | 474 | CZ | TYR | 61 | 4.327 | 25.231 | 98.043 | 1.00 | 25.45 | AAGL |
| ATOM | 475 | OH | TYR | 61 | 4.403 | 26.565 | 97.687 | 1.00 | 24.80 | AAGL |
| ATOM | 476 | C | TYR | 61 | 6.422 | 20.444 | 98.330 | 1.00 | 26.83 | AAGL |
| ATOM | 477 | O | TYR | 61 | 7.039 | 20.948 | 97.393 | 1.00 | 25.72 | AAGL |
| ATOM | 478 | N | ASN | 62 | 6.992 | 20.159 | 99.493 | 1.00 | 24.55 | AAGL |
| ATOM | 479 | CA | ASN | 62 | 8.388 | 20.458 | 99.733 | 1.00 | 25.46 | AAGL |
| ATOM | 480 | CB | ASN | 62 | 8.695 | 20.315 | 101.225 | 1.00 | 25.35 | AAGL |
| ATOM | 481 | CG | ASN | 62 | 8.316 | 21.568 | 102.009 | 1.00 | 25.66 | AAGL |
| ATOM | 482 | OD1 | ASN | 62 | 9.047 | 22.556 | 101.998 | 1.00 | 23.45 | AAGL |
| ATOM | 483 | ND2 | ASN | 62 | 7.159 | 21.539 | 102.666 | 1.00 | 21.77 | AAGL |
| ATOM | 484 | C | ASN | 62 | 9.355 | 19.629 | 98.899 | 1.00 | 25.81 | AAGL |
| ATOM | 485 | O | ASN | 62 | 10.450 | 20.090 | 98.596 | 1.00 | 23.79 | AAGL |
| ATOM | 486 | N | LEU | 63 | 8.969 | 18.411 | 98.528 | 1.00 | 25.79 | AAGL |
| ATOM | 487 | CA | LEU | 63 | 9.856 | 17.589 | 97.708 | 1.00 | 27.44 | AAGL |
| ATOM | 488 | CB | LEU | 63 | 9.320 | 16.153 | 97.581 | 1.00 | 29.01 | AAGL |
| ATOM | 489 | CG | LEU | 63 | 9.673 | 15.225 | 98.743 | 1.00 | 31.95 | AAGL |
| ATOM | 490 | CD1 | LEU | 63 | 9.041 | 13.851 | 98.508 | 1.00 | 32.91 | AAGL |
| ATOM | 491 | CD2 | LEU | 63 | 11.199 | 15.114 | 98.872 | 1.00 | 32.19 | AAGL |
| ATOM | 492 | C | LEU | 63 | 10.001 | 18.207 | 96.322 | 1.00 | 27.90 | AAGL |
| ATOM | 493 | O | LEU | 63 | 11.102 | 18.275 | 95.772 | 1.00 | 29.37 | AAGL |
| ATOM | 494 | N | GLU | 64 | 8.882 | 18.662 | 95.768 | 1.00 | 28.38 | AAGL |
| ATOM | 495 | CA | GLU | 64 | 8.859 | 19.280 | 94.447 | 1.00 | 30.60 | AAGL |
| ATOM | 496 | CB | GLU | 64 | 7.414 | 19.642 | 94.078 | 1.00 | 32.03 | AAGL |
| ATOM | 497 | CG | GLU | 64 | 7.198 | 20.124 | 92.639 | 1.00 | 36.66 | AAGL |
| ATOM | 498 | CD | GLU | 64 | 5.747 | 20.468 | 92.364 | 1.00 | 38.83 | AAGL |
| ATOM | 499 | OE1 | GLU | 64 | 4.874 | 19.637 | 92.688 | 1.00 | 41.75 | AAGL |
| ATOM | 500 | OE2 | GLU | 64 | 5.464 | 21.565 | 91.822 | 1.00 | 41.60 | AAGL |
| ATOM | 501 | C | GLU | 64 | 9.727 | 20.536 | 94.454 | 1.00 | 29.58 | AAGL |
| ATOM | 502 | O | GLU | 64 | 10.525 | 20.769 | 93.541 | 1.00 | 27.18 | AAGL |
| ATOM | 503 | N | LEU | 65 | 9.578 | 21.343 | 95.497 | 1.00 | 27.01 | AAGL |
| ATOM | 504 | CA | LEU | 65 | 10.344 | 22.576 | 95.611 | 1.00 | 25.95 | AAGL |
| ATOM | 505 | CB | LEU | 65 | 9.754 | 23.455 | 96.721 | 1.00 | 27.05 | AAGL |
| ATOM | 506 | CG | LEU | 65 | 10.420 | 24.806 | 97.018 | 1.00 | 25.59 | AAGL |
| ATOM | 507 | CD1 | LEU | 65 | 10.528 | 25.628 | 95.760 | 1.00 | 24.36 | AAGL |
| ATOM | 508 | CD2 | LEU | 65 | 9.600 | 25.544 | 98.074 | 1.00 | 25.15 | AAGL |
| ATOM | 509 | C | LEU | 65 | 11.824 | 22.329 | 95.877 | 1.00 | 26.00 | AAGL |
| ATOM | 510 | O | LEU | 65 | 12.677 | 23.029 | 95.329 | 1.00 | 27.12 | AAGL |
| ATOM | 511 | N | ALA | 66 | 12.131 | 21.330 | 96.699 | 1.00 | 23.38 | AAGL |
| ATOM | 512 | CA | ALA | 66 | 13.517 | 21.025 | 97.038 | 1.00 | 25.19 | AAGL |
| ATOM | 513 | CB | ALA | 66 | 13.572 | 20.017 | 98.203 | 1.00 | 25.90 | AAGL |
| ATOM | 514 | C | ALA | 66 | 14.278 | 20.481 | 95.833 | 1.00 | 27.46 | AAGL |
| ATOM | 515 | O | ALA | 66 | 15.479 | 20.714 | 95.697 | 1.00 | 28.22 | AAGL |
| ATOM | 516 | N | LYS | 67 | 13.578 | 19.752 | 94.969 | 1.00 | 28.70 | AAGL |
| ATOM | 517 | CA | LYS | 67 | 14.201 | 19.188 | 93.768 | 1.00 | 32.17 | AAGL |
| ATOM | 518 | CB | LYS | 67 | 13.164 | 18.444 | 92.924 | 1.00 | 32.68 | AAGL |
| ATOM | 519 | CG | LYS | 67 | 12.902 | 17.003 | 93.358 | 1.00 | 36.34 | AAGL |
| ATOM | 520 | CD | LYS | 67 | 11.676 | 16.443 | 92.655 | 1.00 | 38.14 | AAGL |
| ATOM | 521 | CE | LYS | 67 | 11.447 | 14.989 | 93.012 | 1.00 | 41.38 | AAGL |
| ATOM | 522 | NZ | LYS | 67 | 10.184 | 14.468 | 92.407 | 1.00 | 43.11 | AAGL |
| ATOM | 523 | C | LYS | 67 | 14.813 | 20.303 | 92.931 | 1.00 | 32.63 | AAGL |
| ATOM | 524 | O | LYS | 67 | 15.943 | 20.192 | 92.453 | 1.00 | 32.89 | AAGL |
| ATOM | 525 | N | ARG | 68 | 14.053 | 21.376 | 92.763 | 1.00 | 31.49 | AAGL |
| ATOM | 526 | CA | ARG | 68 | 14.497 | 22.523 | 91.988 | 1.00 | 31.44 | AAGL |
| ATOM | 527 | CB | ARG | 68 | 13.300 | 23.419 | 91.683 | 1.00 | 31.14 | AAGL |

# Fig. 3 cont.

| ATOM | 528 | CG | ARG | 68 | 12.313 | 22.760 | 90.730 | 1.00 | 33.54 | AAGL |
|------|-----|-----|-----|----|--------|--------|--------|------|-------|------|
| ATOM | 529 | CD | ARG | 68 | 11.016 | 23.518 | 90.619 | 1.00 | 32.13 | AAGL |
| ATOM | 530 | NE | ARG | 68 | 11.222 | 24.924 | 90.303 | 1.00 | 31.17 | AAGL |
| ATOM | 531 | CZ | ARG | 68 | 10.238 | 25.763 | 90.002 | 1.00 | 32.92 | AAGL |
| ATOM | 532 | NH1 | ARG | 68 | 8.985 | 25.327 | 89.970 | 1.00 | 33.31 | AAGL |
| ATOM | 533 | NH2 | ARG | 68 | 10.498 | 27.040 | 89.755 | 1.00 | 31.47 | AAGL |
| ATOM | 534 | C | ARG | 68 | 15.595 | 23.311 | 92.691 | 1.00 | 31.54 | AAGL |
| ATOM | 535 | O | ARG | 68 | 16.459 | 23.905 | 92.040 | 1.00 | 31.76 | AAGL |
| ATOM | 536 | N | VAL | 69 | 15.570 | 23.319 | 94.021 | 1.00 | 28.62 | AAGL |
| ATOM | 537 | CA | VAL | 69 | 16.584 | 24.025 | 94.794 | 1.00 | 27.79 | AAGL |
| ATOM | 538 | CB | VAL | 69 | 16.204 | 24.061 | 96.281 | 1.00 | 24.83 | AAGL |
| ATOM | 539 | CG1 | VAL | 69 | 17.294 | 24.735 | 97.092 | 1.00 | 27.63 | AAGL |
| ATOM | 540 | CG2 | VAL | 69 | 14.886 | 24.781 | 96.442 | 1.00 | 26.08 | AAGL |
| ATOM | 541 | C | VAL | 69 | 17.934 | 23.325 | 94.635 | 1.00 | 29.09 | AAGL |
| ATOM | 542 | O | VAL | 69 | 18.968 | 23.970 | 94.458 | 1.00 | 28.64 | AAGL |
| ATOM | 543 | N | LYS | 70 | 17.908 | 21.998 | 94.711 | 1.00 | 29.15 | AAGL |
| ATOM | 544 | CA | LYS | 70 | 19.108 | 21.187 | 94.561 | 1.00 | 31.30 | AAGL |
| ATOM | 545 | CB | LYS | 70 | 18.756 | 19.707 | 94.743 | 1.00 | 34.31 | AAGL |
| ATOM | 546 | CG | LYS | 70 | 19.889 | 18.752 | 94.422 | 1.00 | 36.20 | AAGL |
| ATOM | 547 | CD | LYS | 70 | 19.399 | 17.319 | 94.271 | 1.00 | 40.57 | AAGL |
| ATOM | 548 | CE | LYS | 70 | 18.290 | 17.224 | 93.229 | 1.00 | 41.78 | AAGL |
| ATOM | 549 | NZ | LYS | 70 | 18.666 | 17.932 | 91.966 | 1.00 | 42.36 | AAGL |
| ATOM | 550 | C | LYS | 70 | 19.693 | 21.403 | 93.159 | 1.00 | 31.39 | AAGL |
| ATOM | 551 | O | LYS | 70 | 20.903 | 21.592 | 92.997 | 1.00 | 31.53 | AAGL |
| ATOM | 552 | N | ALA | 71 | 18.813 | 21.386 | 92.165 | 1.00 | 30.10 | AAGL |
| ATOM | 553 | CA | ALA | 71 | 19.196 | 21.564 | 90.771 | 1.00 | 31.78 | AAGL |
| ATOM | 554 | CB | ALA | 71 | 17.957 | 21.525 | 89.879 | 1.00 | 30.31 | AAGL |
| ATOM | 555 | C | ALA | 71 | 19.949 | 22.870 | 90.570 | 1.00 | 33.02 | AAGL |
| ATOM | 556 | O | ALA | 71 | 20.975 | 22.900 | 89.888 | 1.00 | 32.79 | AAGL |
| ATOM | 557 | N | ALA | 72 | 19.442 | 23.940 | 91.179 | 1.00 | 32.06 | AAGL |
| ATOM | 558 | CA | ALA | 72 | 20.054 | 25.257 | 91.071 | 1.00 | 30.23 | AAGL |
| ATOM | 559 | CB | ALA | 72 | 19.048 | 26.323 | 91.463 | 1.00 | 31.29 | AAGL |
| ATOM | 560 | C | ALA | 72 | 21.316 | 25.389 | 91.915 | 1.00 | 29.83 | AAGL |
| ATOM | 561 | O | ALA | 72 | 21.908 | 26.463 | 91.990 | 1.00 | 29.82 | AAGL |
| ATOM | 562 | N | GLY | 73 | 21.714 | 24.298 | 92.561 | 1.00 | 28.89 | AAGL |
| ATOM | 563 | CA | GLY | 73 | 22.926 | 24.304 | 93.360 | 1.00 | 30.91 | AAGL |
| ATOM | 564 | C | GLY | 73 | 22.909 | 25.064 | 94.675 | 1.00 | 32.00 | AAGL |
| ATOM | 565 | O | GLY | 73 | 23.939 | 25.589 | 95.111 | 1.00 | 30.50 | AAGL |
| ATOM | 566 | N | MET | 74 | 21.748 | 25.121 | 95.316 | 1.00 | 31.23 | AAGL |
| ATOM | 567 | CA | MET | 74 | 21.641 | 25.814 | 96.593 | 1.00 | 31.02 | AAGL |
| ATOM | 568 | CB | MET | 74 | 20.500 | 26.840 | 96.537 | 1.00 | 29.51 | AAGL |
| ATOM | 569 | CG | MET | 74 | 20.676 | 27.893 | 95.434 | 1.00 | 29.42 | AAGL |
| ATOM | 570 | SD | MET | 74 | 19.481 | 29.259 | 95.503 | 1.00 | 28.77 | AAGL |
| ATOM | 571 | CE | MET | 74 | 18.129 | 28.654 | 94.532 | 1.00 | 26.24 | AAGL |
| ATOM | 572 | C | MET | 74 | 21.388 | 24.768 | 97.681 | 1.00 | 29.72 | AAGL |
| ATOM | 573 | O | MET | 74 | 20.893 | 23.682 | 97.385 | 1.00 | 30.60 | AAGL |
| ATOM | 574 | N | SER | 75 | 21.750 | 25.075 | 98.925 | 1.00 | 28.06 | AAGL |
| ATOM | 575 | CA | SER | 75 | 21.534 | 24.125 | 100.011 | 1.00 | 25.93 | AAGL |
| ATOM | 576 | CB | SER | 75 | 22.454 | 24.426 | 101.202 | 1.00 | 25.27 | AAGL |
| ATOM | 577 | OG | SER | 75 | 22.281 | 25.752 | 101.671 | 1.00 | 24.77 | AAGL |
| ATOM | 578 | C | SER | 75 | 20.075 | 24.203 | 100.439 | 1.00 | 27.57 | AAGL |
| ATOM | 579 | O | SER | 75 | 19.343 | 25.089 | 99.997 | 1.00 | 26.04 | AAGL |
| ATOM | 580 | N | LEU | 76 | 19.655 | 23.268 | 101.286 | 1.00 | 25.74 | AAGL |
| ATOM | 581 | CA | LEU | 76 | 18.273 | 23.227 | 101.747 | 1.00 | 27.05 | AAGL |
| ATOM | 582 | CB | LEU | 76 | 17.602 | 21.941 | 101.268 | 1.00 | 28.62 | AAGL |
| ATOM | 583 | CG | LEU | 76 | 16.130 | 21.726 | 101.615 | 1.00 | 31.64 | AAGL |
| ATOM | 584 | CD1 | LEU | 76 | 15.268 | 22.677 | 100.772 | 1.00 | 29.51 | AAGL |
| ATOM | 585 | CD2 | LEU | 76 | 15.748 | 20.268 | 101.346 | 1.00 | 32.16 | AAGL |
| ATOM | 586 | C | LEU | 76 | 18.177 | 23.309 | 103.264 | 1.00 | 24.07 | AAGL |
| ATOM | 587 | O | LEU | 76 | 18.890 | 22.619 | 103.985 | 1.00 | 24.81 | AAGL |
| ATOM | 588 | N | TYR | 77 | 17.293 | 24.179 | 103.732 | 1.00 | 24.59 | AAGL |
| ATOM | 589 | CA | TYR | 77 | 17.044 | 24.375 | 105.162 | 1.00 | 21.21 | AAGL |
| ATOM | 590 | CB | TYR | 77 | 17.441 | 25.812 | 105.550 | 1.00 | 21.04 | AAGL |
| ATOM | 591 | CG | TYR | 77 | 16.903 | 26.417 | 106.849 | 1.00 | 22.71 | AAGL |
| ATOM | 592 | CD1 | TYR | 77 | 16.207 | 25.664 | 107.800 | 1.00 | 20.07 | AAGL |
| ATOM | 593 | CE1 | TYR | 77 | 15.681 | 26.276 | 108.959 | 1.00 | 21.30 | AAGL |

# Fig. 3 cont.

| | | | | | | | | | |
|------|-----|-----|-----|----|---------|--------|---------|------|-------|------|
| ATOM | 594 | CD2 | TYR | 77 | 17.069 | 27.784 | 107.091 | 1.00 | 20.07 | AAGL |
| ATOM | 595 | CE2 | TYR | 77 | 16.558 | 28.394 | 108.232 | 1.00 | 22.16 | AAGL |
| ATOM | 596 | CZ | TYR | 77 | 15.863 | 27.646 | 109.159 | 1.00 | 22.47 | AAGL |
| ATOM | 597 | OH | TYR | 77 | 15.331 | 28.312 | 110.248 | 1.00 | 21.22 | AAGL |
| ATOM | 598 | C | TYR | 77 | 15.553 | 24.121 | 105.318 | 1.00 | 19.67 | AAGL |
| ATOM | 599 | O | TYR | 77 | 14.730 | 24.875 | 104.804 | 1.00 | 21.16 | AAGL |
| ATOM | 600 | N | LEU | 78 | 15.217 | 23.021 | 105.989 | 1.00 | 19.73 | AAGL |
| ATOM | 601 | CA | LEU | 78 | 13.826 | 22.662 | 106.216 | 1.00 | 20.07 | AAGL |
| ATOM | 602 | CB | LEU | 78 | 13.645 | 21.140 | 106.164 | 1.00 | 20.48 | AAGL |
| ATOM | 603 | CG | LEU | 78 | 13.793 | 20.485 | 104.784 | 1.00 | 24.57 | AAGL |
| ATOM | 604 | CD1 | LEU | 78 | 13.633 | 18.969 | 104.898 | 1.00 | 25.27 | AAGL |
| ATOM | 605 | CD2 | LEU | 78 | 12.750 | 21.067 | 103.833 | 1.00 | 23.90 | AAGL |
| ATOM | 606 | C | LEU | 78 | 13.379 | 23.199 | 107.568 | 1.00 | 17.57 | AAGL |
| ATOM | 607 | O | LEU | 78 | 13.980 | 22.891 | 108.599 | 1.00 | 18.99 | AAGL |
| ATOM | 608 | N | ASP | 79 | 12.332 | 24.018 | 107.534 | 1.00 | 18.03 | AAGL |
| ATOM | 609 | CA | ASP | 79 | 11.754 | 24.642 | 108.721 | 1.00 | 18.85 | AAGL |
| ATOM | 610 | CB | ASP | 79 | 11.386 | 26.098 | 108.389 | 1.00 | 19.55 | AAGL |
| ATOM | 611 | CG | ASP | 79 | 10.593 | 26.785 | 109.493 | 1.00 | 25.39 | AAGL |
| ATOM | 612 | OD1 | ASP | 79 | 10.682 | 26.370 | 110.662 | 1.00 | 22.47 | AAGL |
| ATOM | 613 | OD2 | ASP | 79 | 9.885 | 27.761 | 109.180 | 1.00 | 27.84 | AAGL |
| ATOM | 614 | C | ASP | 79 | 10.514 | 23.848 | 109.116 | 1.00 | 16.61 | AAGL |
| ATOM | 615 | O | ASP | 79 | 9.427 | 24.105 | 108.608 | 1.00 | 16.77 | AAGL |
| ATOM | 616 | N | LEU | 80 | 10.686 | 22.881 | 110.014 | 1.00 | 16.76 | AAGL |
| ATOM | 617 | CA | LEU | 80 | 9.573 | 22.051 | 110.452 | 1.00 | 17.99 | AAGL |
| ATOM | 618 | CB | LEU | 80 | 10.077 | 20.777 | 111.132 | 1.00 | 18.64 | AAGL |
| ATOM | 619 | CG | LEU | 80 | 11.103 | 19.918 | 110.385 | 1.00 | 19.36 | AAGL |
| ATOM | 620 | CD1 | LEU | 80 | 11.345 | 18.636 | 111.166 | 1.00 | 20.62 | AAGL |
| ATOM | 621 | CD2 | LEU | 80 | 10.603 | 19.605 | 108.986 | 1.00 | 18.29 | AAGL |
| ATOM | 622 | C | LEU | 80 | 8.708 | 22.802 | 111.441 | 1.00 | 18.46 | AAGL |
| ATOM | 623 | O | LEU | 80 | 9.162 | 23.121 | 112.529 | 1.00 | 20.06 | AAGL |
| ATOM | 624 | N | HIS | 81 | 7.464 | 23.086 | 111.071 | 1.00 | 17.32 | AAGL |
| ATOM | 625 | CA | HIS | 81 | 6.572 | 23.780 | 111.987 | 1.00 | 16.30 | AAGL |
| ATOM | 626 | CB | HIS | 81 | 5.475 | 24.525 | 111.223 | 1.00 | 15.62 | AAGL |
| ATOM | 627 | CG | HIS | 81 | 5.939 | 25.810 | 110.612 | 1.00 | 19.94 | AAGL |
| ATOM | 628 | CD2 | HIS | 81 | 7.137 | 26.167 | 110.093 | 1.00 | 19.51 | AAGL |
| ATOM | 629 | ND1 | HIS | 81 | 5.129 | 26.921 | 110.507 | 1.00 | 20.10 | AAGL |
| ATOM | 630 | CE1 | HIS | 81 | 5.811 | 27.909 | 109.952 | 1.00 | 20.61 | AAGL |
| ATOM | 631 | NE2 | HIS | 81 | 7.031 | 27.477 | 109.693 | 1.00 | 20.38 | AAGL |
| ATOM | 632 | C | HIS | 81 | 5.939 | 22.811 | 112.984 | 1.00 | 17.32 | AAGL |
| ATOM | 633 | O | HIS | 81 | 5.368 | 23.240 | 113.987 | 1.00 | 18.88 | AAGL |
| ATOM | 634 | N | LEU | 82 | 6.045 | 21.513 | 112.709 | 1.00 | 16.02 | AAGL |
| ATOM | 635 | CA | LEU | 82 | 5.484 | 20.480 | 113.588 | 1.00 | 17.14 | AAGL |
| ATOM | 636 | CB | LEU | 82 | 6.339 | 20.342 | 114.850 | 1.00 | 16.85 | AAGL |
| ATOM | 637 | CG | LEU | 82 | 7.813 | 20.007 | 114.595 | 1.00 | 20.75 | AAGL |
| ATOM | 638 | CD1 | LEU | 82 | 8.537 | 19.890 | 115.923 | 1.00 | 18.12 | AAGL |
| ATOM | 639 | CD2 | LEU | 82 | 7.935 | 18.712 | 113.812 | 1.00 | 18.95 | AAGL |
| ATOM | 640 | C | LEU | 82 | 4.048 | 20.826 | 113.965 | 1.00 | 18.59 | AAGL |
| ATOM | 641 | O | LEU | 82 | 3.664 | 20.829 | 115.146 | 1.00 | 18.40 | AAGL |
| ATOM | 642 | N | SER | 83 | 3.268 | 21.109 | 112.930 | 1.00 | 16.93 | AAGL |
| ATOM | 643 | CA | SER | 83 | 1.868 | 21.475 | 113.052 | 1.00 | 16.95 | AAGL |
| ATOM | 644 | CB | SER | 83 | 1.757 | 22.914 | 113.569 | 1.00 | 17.01 | AAGL |
| ATOM | 645 | OG | SER | 83 | 0.415 | 23.351 | 113.629 | 1.00 | 17.93 | AAGL |
| ATOM | 646 | C | SER | 83 | 1.276 | 21.367 | 111.649 | 1.00 | 18.89 | AAGL |
| ATOM | 647 | O | SER | 83 | 2.011 | 21.239 | 110.664 | 1.00 | 19.84 | AAGL |
| ATOM | 648 | N | ASP | 84 | -0.046 | 21.404 | 111.561 | 1.00 | 19.63 | AAGL |
| ATOM | 649 | CA | ASP | 84 | -0.715 | 21.317 | 110.275 | 1.00 | 20.59 | AAGL |
| ATOM | 650 | CB | ASP | 84 | -2.107 | 20.695 | 110.421 | 1.00 | 22.19 | AAGL |
| ATOM | 651 | CG | ASP | 84 | -2.062 | 19.246 | 110.817 | 1.00 | 21.52 | AAGL |
| ATOM | 652 | OD1 | ASP | 84 | -1.025 | 18.597 | 110.572 | 1.00 | 23.10 | AAGL |
| ATOM | 653 | OD2 | ASP | 84 | -3.079 | 18.755 | 111.360 | 1.00 | 23.55 | AAGL |
| ATOM | 654 | C | ASP | 84 | -0.866 | 22.706 | 109.689 | 1.00 | 21.71 | AAGL |
| ATOM | 655 | O | ASP | 84 | -1.340 | 22.854 | 108.563 | 1.00 | 21.81 | AAGL |
| ATOM | 656 | N | THR | 85 | -0.461 | 23.717 | 110.453 | 1.00 | 21.01 | AAGL |
| ATOM | 657 | CA | THR | 85 | -0.573 | 25.102 | 110.012 | 1.00 | 19.92 | AAGL |
| ATOM | 658 | CB | THR | 85 | -1.971 | 25.670 | 110.370 | 1.00 | 22.17 | AAGL |
| ATOM | 659 | OG1 | THR | 85 | -2.144 | 26.952 | 109.763 | 1.00 | 22.62 | AAGL |

# Fig. 3 cont.

| ATOM | 660 | CG2 | THR | 85 | -2.134 | 25.800 | 111.874 | 1.00 | 23.94 | AAGL |
|------|-----|-----|-----|----|--------|--------|---------|------|-------|------|
| ATOM | 661 | C | THR | 85 | 0.527 | 25.958 | 110.646 | 1.00 | 19.33 | AAGL |
| ATOM | 662 | O | THR | 85 | 1.429 | 25.425 | 111.298 | 1.00 | 18.85 | AAGL |
| ATOM | 663 | N | TRP | 86 | 0.454 | 27.276 | 110.450 | 1.00 | 18.81 | AAGL |
| ATOM | 664 | CA | TRP | 86 | 1.455 | 28.199 | 110.988 | 1.00 | 17.88 | AAGL |
| ATOM | 665 | CB | TRP | 86 | 1.011 | 29.654 | 110.800 | 1.00 | 17.85 | AAGL |
| ATOM | 666 | CG | TRP | 86 | 0.672 | 30.016 | 109.399 | 1.00 | 18.75 | AAGL |
| ATOM | 667 | CD2 | TRP | 86 | 1.587 | 30.427 | 108.382 | 1.00 | 18.96 | AAGL |
| ATOM | 668 | CE2 | TRP | 86 | 0.832 | 30.649 | 107.209 | 1.00 | 21.98 | AAGL |
| ATOM | 669 | CE3 | TRP | 86 | 2.975 | 30.628 | 108.345 | 1.00 | 18.78 | AAGL |
| ATOM | 670 | CD1 | TRP | 86 | -0.563 | 30.004 | 108.826 | 1.00 | 21.00 | AAGL |
| ATOM | 671 | NE1 | TRP | 86 | -0.478 | 30.386 | 107.508 | 1.00 | 21.68 | AAGL |
| ATOM | 672 | CZ2 | TRP | 86 | 1.418 | 31.065 | 106.007 | 1.00 | 19.73 | AAGL |
| ATOM | 673 | CZ3 | TRP | 86 | 3.556 | 31.041 | 107.151 | 1.00 | 20.30 | AAGL |
| ATOM | 674 | CH2 | TRP | 86 | 2.775 | 31.255 | 105.998 | 1.00 | 18.40 | AAGL |
| ATOM | 675 | C | TRP | 86 | 1.757 | 27.994 | 112.467 | 1.00 | 18.54 | AAGL |
| ATOM | 676 | O | TRP | 86 | 0.847 | 27.998 | 113.302 | 1.00 | 17.68 | AAGL |
| ATOM | 677 | N | ALA | 87 | 3.035 | 27.830 | 112.793 | 1.00 | 15.65 | AAGL |
| ATOM | 678 | CA | ALA | 87 | 3.440 | 27.669 | 114.182 | 1.00 | 19.55 | AAGL |
| ATOM | 679 | CB | ALA | 87 | 4.263 | 26.393 | 114.355 | 1.00 | 17.55 | AAGL |
| ATOM | 680 | C | ALA | 87 | 4.266 | 28.880 | 114.613 | 1.00 | 17.89 | AAGL |
| ATOM | 681 | O | ALA | 87 | 5.179 | 29.303 | 113.896 | 1.00 | 18.09 | AAGL |
| ATOM | 682 | N | ASP | 88 | 3.933 | 29.441 | 115.772 | 1.00 | 18.18 | AAGL |
| ATOM | 683 | CA | ASP | 88 | 4.655 | 30.585 | 116.325 | 1.00 | 18.94 | AAGL |
| ATOM | 684 | CB | ASP | 88 | 4.276 | 31.885 | 115.604 | 1.00 | 21.76 | AAGL |
| ATOM | 685 | CG | ASP | 88 | 2.798 | 32.205 | 115.699 | 1.00 | 26.60 | AAGL |
| ATOM | 686 | OD1 | ASP | 88 | 2.221 | 32.074 | 116.789 | 1.00 | 24.49 | AAGL |
| ATOM | 687 | OD2 | ASP | 88 | 2.216 | 32.599 | 114.673 | 1.00 | 30.64 | AAGL |
| ATOM | 688 | C | ASP | 88 | 4.349 | 30.674 | 117.826 | 1.00 | 20.25 | AAGL |
| ATOM | 689 | O | ASP | 88 | 3.617 | 29.838 | 118.354 | 1.00 | 18.36 | AAGL |
| ATOM | 690 | N | PRO | 89 | 4.900 | 31.681 | 118.528 | 1.00 | 19.03 | AAGL |
| ATOM | 691 | CD | PRO | 89 | 5.879 | 32.685 | 118.078 | 1.00 | 20.41 | AAGL |
| ATOM | 692 | CA | PRO | 89 | 4.656 | 31.813 | 119.969 | 1.00 | 19.78 | AAGL |
| ATOM | 693 | CB | PRO | 89 | 5.435 | 33.071 | 120.339 | 1.00 | 22.34 | AAGL |
| ATOM | 694 | CG | PRO | 89 | 6.561 | 33.059 | 119.354 | 1.00 | 20.37 | AAGL |
| ATOM | 695 | C | PRO | 89 | 3.206 | 31.882 | 120.421 | 1.00 | 21.51 | AAGL |
| ATOM | 696 | O | PRO | 89 | 2.909 | 31.593 | 121.578 | 1.00 | 22.07 | AAGL |
| ATOM | 697 | N | SER | 90 | 2.297 | 32.251 | 119.527 | 1.00 | 20.56 | AAGL |
| ATOM | 698 | CA | SER | 90 | 0.904 | 32.335 | 119.924 | 1.00 | 21.51 | AAGL |
| ATOM | 699 | CB | SER | 90 | 0.283 | 33.644 | 119.425 | 1.00 | 24.67 | AAGL |
| ATOM | 700 | OG | SER | 90 | 0.139 | 33.643 | 118.023 | 1.00 | 29.17 | AAGL |
| ATOM | 701 | C | SER | 90 | 0.086 | 31.138 | 119.451 | 1.00 | 21.66 | AAGL |
| ATOM | 702 | O | SER | 90 | -1.094 | 31.018 | 119.792 | 1.00 | 18.80 | AAGL |
| ATOM | 703 | N | ASP | 91 | 0.710 | 30.249 | 118.674 | 1.00 | 19.99 | AAGL |
| ATOM | 704 | CA | ASP | 91 | 0.025 | 29.052 | 118.188 | 1.00 | 21.82 | AAGL |
| ATOM | 705 | CB | ASP | 91 | -0.839 | 29.374 | 116.961 | 1.00 | 26.37 | AAGL |
| ATOM | 706 | CG | ASP | 91 | -2.057 | 30.208 | 117.305 | 0.50 | 27.60 | AAGL |
| ATOM | 707 | OD1 | ASP | 91 | -2.904 | 29.743 | 118.104 | 0.50 | 29.99 | AAGL |
| ATOM | 708 | OD2 | ASP | 91 | -2.168 | 31.328 | 116.770 | 0.50 | 29.72 | AAGL |
| ATOM | 709 | C | ASP | 91 | 0.974 | 27.912 | 117.816 | 1.00 | 19.33 | AAGL |
| ATOM | 710 | O | ASP | 91 | 1.713 | 27.997 | 116.834 | 1.00 | 20.80 | AAGL |
| ATOM | 711 | N | GLN | 92 | 0.945 | 26.851 | 118.614 | 1.00 | 16.40 | AAGL |
| ATOM | 712 | CA | GLN | 92 | 1.751 | 25.653 | 118.369 | 1.00 | 17.43 | AAGL |
| ATOM | 713 | CB | GLN | 92 | 2.820 | 25.482 | 119.449 | 1.00 | 16.72 | AAGL |
| ATOM | 714 | CG | GLN | 92 | 3.897 | 26.562 | 119.457 | 1.00 | 15.88 | AAGL |
| ATOM | 715 | CD | GLN | 92 | 4.894 | 26.427 | 118.319 | 1.00 | 16.69 | AAGL |
| ATOM | 716 | OE1 | GLN | 92 | 5.078 | 25.345 | 117.770 | 1.00 | 18.84 | AAGL |
| ATOM | 717 | NE2 | GLN | 92 | 5.550 | 27.524 | 117.970 | 1.00 | 15.00 | AAGL |
| ATOM | 718 | C | GLN | 92 | 0.782 | 24.472 | 118.403 | 1.00 | 17.98 | AAGL |
| ATOM | 719 | O | GLN | 92 | 0.855 | 23.615 | 119.284 | 1.00 | 18.87 | AAGL |
| ATOM | 720 | N | THR | 93 | -0.140 | 24.444 | 117.450 | 1.00 | 18.32 | AAGL |
| ATOM | 721 | CA | THR | 93 | -1.137 | 23.378 | 117.396 | 1.00 | 19.90 | AAGL |
| ATOM | 722 | CB | THR | 93 | -2.303 | 23.732 | 116.451 | 1.00 | 21.83 | AAGL |
| ATOM | 723 | OG1 | THR | 93 | -2.845 | 25.001 | 116.824 | 1.00 | 23.30 | AAGL |
| ATOM | 724 | CG2 | THR | 93 | -3.415 | 22.691 | 116.564 | 1.00 | 23.34 | AAGL |
| ATOM | 725 | C | THR | 93 | -0.553 | 22.052 | 116.946 | 1.00 | 19.51 | AAGL |

# Fig. 3 cont.

| ATOM | 726 | O   | THR | 93  | 0.000  | 21.935 | 115.856 | 1.00 | 19.99 | AAGL |
|------|-----|-----|-----|-----|--------|--------|---------|------|-------|------|
| ATOM | 727 | N   | THR | 94  | -0.685 | 21.050 | 117.802 | 1.00 | 19.55 | AAGL |
| ATOM | 728 | CA  | THR | 94  | -0.181 | 19.716 | 117.510 | 1.00 | 20.32 | AAGL |
| ATOM | 729 | CB  | THR | 94  | -0.463 | 18.775 | 118.699 | 1.00 | 20.34 | AAGL |
| ATOM | 730 | OG1 | THR | 94  | 0.320  | 19.190 | 119.824 | 1.00 | 20.72 | AAGL |
| ATOM | 731 | CG2 | THR | 94  | -0.141 | 17.334 | 118.348 | 1.00 | 20.41 | AAGL |
| ATOM | 732 | C   | THR | 94  | -0.866 | 19.171 | 116.261 | 1.00 | 19.20 | AAGL |
| ATOM | 733 | O   | THR | 94  | -2.060 | 19.367 | 116.071 | 1.00 | 19.04 | AAGL |
| ATOM | 734 | N   | PRO | 95  | -0.111 | 18.495 | 115.381 | 1.00 | 19.53 | AAGL |
| ATOM | 735 | CD  | PRO | 95  | 1.352  | 18.315 | 115.386 | 1.00 | 17.38 | AAGL |
| ATOM | 736 | CA  | PRO | 95  | -0.703 | 17.937 | 114.160 | 1.00 | 20.73 | AAGL |
| ATOM | 737 | CB  | PRO | 95  | 0.424  | 17.086 | 113.590 | 1.00 | 16.98 | AAGL |
| ATOM | 738 | CG  | PRO | 95  | 1.638  | 17.872 | 113.952 | 1.00 | 20.07 | AAGL |
| ATOM | 739 | C   | PRO | 95  | -1.939 | 17.091 | 114.452 | 1.00 | 22.21 | AAGL |
| ATOM | 740 | O   | PRO | 95  | -2.002 | 16.399 | 115.468 | 1.00 | 19.37 | AAGL |
| ATOM | 741 | N   | SER | 96  | -2.926 | 17.163 | 113.569 | 1.00 | 23.26 | AAGL |
| ATOM | 742 | CA  | SER | 96  | -4.125 | 16.353 | 113.740 | 1.00 | 27.34 | AAGL |
| ATOM | 743 | CB  | SER | 96  | -5.153 | 16.695 | 112.656 | 1.00 | 29.38 | AAGL |
| ATOM | 744 | OG  | SER | 96  | -4.577 | 16.561 | 111.365 | 1.00 | 34.62 | AAGL |
| ATOM | 745 | C   | SER | 96  | -3.635 | 14.911 | 113.590 | 1.00 | 28.07 | AAGL |
| ATOM | 746 | O   | SER | 96  | -2.863 | 14.602 | 112.685 | 1.00 | 29.54 | AAGL |
| ATOM | 747 | N   | GLY | 97  | -4.064 | 14.029 | 114.482 | 1.00 | 28.91 | AAGL |
| ATOM | 748 | CA  | GLY | 97  | -3.607 | 12.655 | 114.390 | 1.00 | 28.58 | AAGL |
| ATOM | 749 | C   | GLY | 97  | -2.478 | 12.365 | 115.365 | 1.00 | 27.25 | AAGL |
| ATOM | 750 | O   | GLY | 97  | -2.214 | 11.202 | 115.679 | 1.00 | 28.56 | AAGL |
| ATOM | 751 | N   | TRP | 98  | -1.786 | 13.408 | 115.819 | 1.00 | 23.62 | AAGL |
| ATOM | 752 | CA  | TRP | 98  | -0.715 | 13.227 | 116.801 | 1.00 | 20.63 | AAGL |
| ATOM | 753 | CB  | TRP | 98  | 0.396  | 14.250 | 116.590 | 1.00 | 20.68 | AAGL |
| ATOM | 754 | CG  | TRP | 98  | 1.253  | 13.995 | 115.382 | 1.00 | 20.26 | AAGL |
| ATOM | 755 | CD2 | TRP | 98  | 2.561  | 14.517 | 115.148 | 1.00 | 19.57 | AAGL |
| ATOM | 756 | CE2 | TRP | 98  | 2.945  | 14.123 | 113.845 | 1.00 | 20.94 | AAGL |
| ATOM | 757 | CE3 | TRP | 98  | 3.449  | 15.288 | 115.913 | 1.00 | 19.61 | AAGL |
| ATOM | 758 | CD1 | TRP | 98  | 0.905  | 13.311 | 114.246 | 1.00 | 21.24 | AAGL |
| ATOM | 759 | NE1 | TRP | 98  | 1.918  | 13.386 | 113.318 | 1.00 | 21.31 | AAGL |
| ATOM | 760 | CZ2 | TRP | 98  | 4.178  | 14.475 | 113.290 | 1.00 | 20.47 | AAGL |
| ATOM | 761 | CZ3 | TRP | 98  | 4.675  | 15.638 | 115.362 | 1.00 | 20.55 | AAGL |
| ATOM | 762 | CH2 | TRP | 98  | 5.028  | 15.230 | 114.058 | 1.00 | 21.24 | AAGL |
| ATOM | 763 | C   | TRP | 98  | -1.348 | 13.397 | 118.190 | 1.00 | 21.31 | AAGL |
| ATOM | 764 | O   | TRP | 98  | -2.422 | 13.973 | 118.312 | 1.00 | 21.68 | AAGL |
| ATOM | 765 | N   | SER | 99  | -0.675 | 12.910 | 119.227 | 1.00 | 22.27 | AAGL |
| ATOM | 766 | CA  | SER | 99  | -1.210 | 12.951 | 120.591 | 1.00 | 20.04 | AAGL |
| ATOM | 767 | CB  | SER | 99  | -0.531 | 11.870 | 121.446 | 1.00 | 21.78 | AAGL |
| ATOM | 768 | OG  | SER | 99  | -1.115 | 11.794 | 122.746 | 1.00 | 19.99 | AAGL |
| ATOM | 769 | C   | SER | 99  | -1.172 | 14.262 | 121.377 | 1.00 | 20.81 | AAGL |
| ATOM | 770 | O   | SER | 99  | -0.174 | 14.974 | 121.391 | 1.00 | 20.17 | AAGL |
| ATOM | 771 | N   | THR | 100 | -2.284 | 14.555 | 122.039 | 1.00 | 21.47 | AAGL |
| ATOM | 772 | CA  | THR | 100 | -2.401 | 15.730 | 122.896 | 1.00 | 22.60 | AAGL |
| ATOM | 773 | CB  | THR | 100 | -3.564 | 16.655 | 122.455 | 1.00 | 22.41 | AAGL |
| ATOM | 774 | OG1 | THR | 100 | -4.759 | 15.882 | 122.308 | 1.00 | 23.06 | AAGL |
| ATOM | 775 | CG2 | THR | 100 | -3.248 | 17.339 | 121.128 | 1.00 | 22.11 | AAGL |
| ATOM | 776 | C   | THR | 100 | -2.706 | 15.190 | 124.294 | 1.00 | 23.80 | AAGL |
| ATOM | 777 | O   | THR | 100 | -3.150 | 15.930 | 125.174 | 1.00 | 23.03 | AAGL |
| ATOM | 778 | N   | THR | 101 | -2.448 | 13.895 | 124.488 | 1.00 | 24.54 | AAGL |
| ATOM | 779 | CA  | THR | 101 | -2.737 | 13.228 | 125.755 | 1.00 | 23.47 | AAGL |
| ATOM | 780 | CB  | THR | 101 | -4.055 | 12.440 | 125.638 | 1.00 | 24.48 | AAGL |
| ATOM | 781 | OG1 | THR | 101 | -3.897 | 11.412 | 124.652 | 1.00 | 25.27 | AAGL |
| ATOM | 782 | CG2 | THR | 101 | -5.198 | 13.356 | 125.213 | 1.00 | 25.93 | AAGL |
| ATOM | 783 | C   | THR | 101 | -1.679 | 12.256 | 126.301 | 1.00 | 25.35 | AAGL |
| ATOM | 784 | O   | THR | 101 | -1.794 | 11.802 | 127.437 | 1.00 | 25.05 | AAGL |
| ATOM | 785 | N   | ASP | 102 | -0.657 | 11.932 | 125.513 | 1.00 | 23.02 | AAGL |
| ATOM | 786 | CA  | ASP | 102 | 0.366  | 10.989 | 125.968 | 1.00 | 24.03 | AAGL |
| ATOM | 787 | CB  | ASP | 102 | 0.013  | 9.579  | 125.488 | 1.00 | 25.87 | AAGL |
| ATOM | 788 | CG  | ASP | 102 | 0.934  | 8.515  | 126.052 | 1.00 | 29.80 | AAGL |
| ATOM | 789 | OD1 | ASP | 102 | 2.163  | 8.600  | 125.864 | 1.00 | 30.75 | AAGL |
| ATOM | 790 | OD2 | ASP | 102 | 0.425  | 7.571  | 126.683 | 1.00 | 35.27 | AAGL |
| ATOM | 791 | C   | ASP | 102 | 1.746  | 11.370 | 125.446 | 1.00 | 24.10 | AAGL |
| ATOM | 792 | O   | ASP | 102 | 2.005  | 11.269 | 124.245 | 1.00 | 24.23 | AAGL |

# Fig. 3 cont.

| ATOM | 793 | N   | LEU | 103 | 2.640  | 11.791 | 126.338 | 1.00 | 23.33 | AAGL  |
|------|-----|-----|-----|-----|--------|--------|---------|------|-------|-------|
| ATOM | 794 | CA  | LEU | 103 | 3.974  | 12.189 | 125.898 | 1.00 | 23.77 | AAGL  |
| ATOM | 795 | CB  | LEU | 103 | 4.801  | 12.749 | 127.056 | 1.00 | 24.26 | AAGL  |
| ATOM | 796 | CG  | LEU | 103 | 6.113  | 13.383 | 126.579 | 1.00 | 23.41 | AAGL  |
| ATOM | 797 | CD1 | LEU | 103 | 5.800  | 14.627 | 125.765 | 1.00 | 23.25 | AAGL  |
| ATOM | 798 | CD2 | LEU | 103 | 7.005  | 13.729 | 127.764 | 1.00 | 24.01 | AAGL  |
| ATOM | 799 | C   | LEU | 103 | 4.744  | 11.046 | 125.257 | 1.00 | 24.93 | AAGL  |
| ATOM | 800 | O   | LEU | 103 | 5.522  | 11.259 | 124.326 | 1.00 | 22.87 | AAGL  |
| ATOM | 801 | N   | GLY | 104 | 4.535  | 9.837  | 125.765 | 1.00 | 24.55 | AAGL  |
| ATOM | 802 | CA  | GLY | 104 | 5.229  | 8.689  | 125.213 | 1.00 | 25.67 | AAGL  |
| ATOM | 803 | C   | GLY | 104 | 4.863  | 8.514  | 123.757 | 1.00 | 24.34 | AAGL  |
| ATOM | 804 | O   | GLY | 104 | 5.727  | 8.334  | 122.899 | 1.00 | 25.72 | AAGL  |
| ATOM | 805 | N   | THR | 105 | 3.571  | 8.571  | 123.475 | 1.00 | 23.33 | AAGL  |
| ATOM | 806 | CA  | THR | 105 | 3.084  | 8.425  | 122.115 | 1.00 | 24.93 | AAGL  |
| ATOM | 807 | CB  | THR | 105 | 1.546  | 8.360  | 122.095 | 1.00 | 25.14 | AAGL  |
| ATOM | 808 | OG1 | THR | 105 | 1.109  | 7.236  | 122.870 | 1.00 | 28.55 | AAGL  |
| ATOM | 809 | CG2 | THR | 105 | 1.029  | 8.211  | 120.684 | 1.00 | 27.78 | AAGL· |
| ATOM | 810 | C   | THR | 105 | 3.561  | 9.596  | 121.260 | 1.00 | 23.97 | AAGL  |
| ATOM | 811 | O   | THR | 105 | 4.008  | 9.412  | 120.132 | 1.00 | 24.40 | AAGL  |
| ATOM | 812 | N   | LEU | 106 | 3.485  | 10.802 | 121.812 | 1.00 | 22.92 | AAGL  |
| ATOM | 813 | CA  | LEU | 106 | 3.898  | 12.000 | 121.085 | 1.00 | 21.38 | AAGL  |
| ATOM | 814 | CB  | LEU | 106 | 3.568  | 13.254 | 121.896 | 1.00 | 19.99 | AAGL  |
| ATOM | 815 | CG  | LEU | 106 | 3.895  | 14.579 | 121.196 | 1.00 | 18.13 | AAGL  |
| ATOM | 816 | CD1 | LEU | 106 | 3.066  | 14.714 | 119.923 | 1.00 | 16.54 | AAGL  |
| ATOM | 817 | CD2 | LEU | 106 | 3.613  | 15.735 | 122.141 | 1.00 | 15.43 | AAGL  |
| ATOM | 818 | C   | LEU | 106 | 5.382  | 11.995 | 120.729 | 1.00 | 23.00 | AAGL  |
| ATOM | 819 | O   | LEU | 106 | 5.755  | 12.330 | 119.601 | 1.00 | 22.17 | AAGL  |
| ATOM | 820 | N   | LYS | 107 | 6.230  | 11.627 | 121.684 | 1.00 | 23.39 | AAGL  |
| ATOM | 821 | CA  | LYS | 107 | 7.662  | 11.578 | 121.420 | 1.00 | 24.69 | AAGL  |
| ATOM | 822 | CB  | LYS | 107 | 8.446  | 11.129 | 122.660 | 1.00 | 25.78 | AAGL  |
| ATOM | 823 | CG  | LYS | 107 | 8.496  | 12.144 | 123.789 | 1.00 | 27.94 | AAGL  |
| ATOM | 824 | CD  | LYS | 107 | 9.574  | 11.781 | 124.801 | 1.00 | 31.83 | AAGL  |
| ATOM | 825 | CE  | LYS | 107 | 9.360  | 10.393 | 125.384 | 1.00 | 36.44 | AAGL  |
| ATOM | 826 | NZ  | LYS | 107 | 10.431 | 10.009 | 126.355 | 1.00 | 39.34 | AAGL  |
| ATOM | 827 | C   | LYS | 107 | 7.942  | 10.609 | 120.278 | 1.00 | 24.60 | AAGL  |
| ATOM | 828 | O   | LYS | 107 | 8.829  | 10.852 | 119.461 | 1.00 | 24.29 | AAGL  |
| ATOM | 829 | N   | TRP | 108 | 7.183  | 9.518  | 120.220 | 1.00 | 24.58 | AAGL  |
| ATOM | 830 | CA  | TRP | 108 | 7.372  | 8.526  | 119.165 | 1.00 | 26.57 | AAGL  |
| ATOM | 831 | CB  | TRP | 108 | 6.616  | 7.231  | 119.487 | 1.00 | 30.79 | AAGL  |
| ATOM | 832 | CG  | TRP | 108 | 7.429  | 6.243  | 120.257 | 1.00 | 37.55 | AAGL  |
| ATOM | 833 | CD2 | TRP | 108 | 8.617  | 5.579  | 119.806 | 1.00 | 41.19 | AAGL  |
| ATOM | 834 | CE2 | TRP | 108 | 9.055  | 4.744  | 120.861 | 1.00 | 41.70 | AAGL  |
| ATOM | 835 | CE3 | TRP | 108 | 9.356  | 5.610  | 118.611 | 1.00 | 40.79 | AAGL  |
| ATOM | 836 | CD1 | TRP | 108 | 7.199  | 5.797  | 121.530 | 1.00 | 39.67 | AAGL  |
| ATOM | 837 | NE1 | TRP | 108 | 8.173  | 4.898  | 121.899 | 1.00 | 41.76 | AAGL  |
| ATOM | 838 | CZ2 | TRP | 108 | 10.202 | 3.942  | 120.760 | 1.00 | 42.41 | AAGL  |
| ATOM | 839 | CZ3 | TRP | 108 | 10.498 | 4.814  | 118.510 | 1.00 | 42.96 | AAGL  |
| ATOM | 840 | CH2 | TRP | 108 | 10.908 | 3.992  | 119.582 | 1.00 | 43.14 | AAGL  |
| ATOM | 841 | C   | TRP | 108 | 6.925  | 9.040  | 117.807 | 1.00 | 25.36 | AAGL  |
| ATOM | 842 | O   | TRP | 108 | 7.585  | 8.785  | 116.801 | 1.00 | 25.01 | AAGL  |
| ATOM | 843 | N   | GLN | 109 | 5.808  | 9.763  | 117.782 | 1.00 | 22.63 | AAGL  |
| ATOM | 844 | CA  | GLN | 109 | 5.277  | 10.304 | 116.539 | 1.00 | 22.94 | AAGL  |
| ATOM | 845 | CB  | GLN | 109 | 3.884  | 10.886 | 116.784 | 1.00 | 22.73 | AAGL  |
| ATOM | 846 | CG  | GLN | 109 | 2.863  | 9.838  | 117.229 | 1.00 | 24.36 | AAGL  |
| ATOM | 847 | CD  | GLN | 109 | 1.555  | 10.447 | 117.706 | 1.00 | 25.79 | AAGL  |
| ATOM | 848 | OE1 | GLN | 109 | 1.551  | 11.462 | 118.410 | 1.00 | 25.25 | AAGL  |
| ATOM | 849 | NE2 | GLN | 109 | 0.434  | 9.821  | 117.340 | 1.00 | 24.06 | AAGL  |
| ATOM | 850 | C   | GLN | 109 | 6.212  | 11.362 | 115.958 | 1.00 | 22.81 | AAGL  |
| ATOM | 851 | O   | GLN | 109 | 6.416  | 11.418 | 114.747 | 1.00 | 23.48 | AAGL  |
| ATOM | 852 | N   | LEU | 110 | 6.796  | 12.181 | 116.826 | 1.00 | 23.23 | AAGL  |
| ATOM | 853 | CA  | LEU | 110 | 7.716  | 13.223 | 116.389 | 1.00 | 23.80 | AAGL  |
| ATOM | 854 | CB  | LEU | 110 | 8.031  | 14.188 | 117.539 | 1.00 | 24.37 | AAGL  |
| ATOM | 855 | CG  | LEU | 110 | 9.119  | 15.231 | 117.255 | 1.00 | 22.16 | AAGL  |
| ATOM | 856 | CD1 | LEU | 110 | 8.792  | 15.973 | 115.960 | 1.00 | 22.25 | AAGL  |
| ATOM | 857 | CD2 | LEU | 110 | 9.230  | 16.199 | 118.420 | 1.00 | 23.11 | AAGL  |
| ATOM | 858 | C   | LEU | 110 | 9.005  | 12.596 | 115.870 | 1.00 | 25.82 | AAGL  |
| ATOM | 859 | O   | LEU | 110 | 9.523  | 13.010 | 114.835 | 1.00 | 24.35 | AAGL  |

**Fig. 3 cont.**

| ATOM | 860 | N   | TYR | 111 | 9.524  | 11.608 | 116.594 | 1.00 | 25.68 | AAGL |
|------|-----|-----|-----|-----|--------|--------|---------|------|-------|------|
| ATOM | 861 | CA  | TYR | 111 | 10.746 | 10.915 | 116.179 | 1.00 | 24.78 | AAGL |
| ATOM | 862 | CB  | TYR | 111 | 11.151 | 9.869  | 117.230 | 1.00 | 25.83 | AAGL |
| ATOM | 863 | CG  | TYR | 111 | 12.199 | 8.874  | 116.767 | 1.00 | 27.35 | AAGL |
| ATOM | 864 | CD1 | TYR | 111 | 11.848 | 7.774  | 115.986 | 1.00 | 29.55 | AAGL |
| ATOM | 865 | CE1 | TYR | 111 | 12.810 | 6.866  | 115.544 | 1.00 | 31.93 | AAGL |
| ATOM | 866 | CD2 | TYR | 111 | 13.541 | 9.043  | 117.099 | 1.00 | 28.41 | AAGL |
| ATOM | 867 | CE2 | TYR | 111 | 14.514 | 8.143  | 116.661 | 1.00 | 32.12 | AAGL |
| ATOM | 868 | CZ  | TYR | 111 | 14.143 | 7.060  | 115.882 | 1.00 | 31.55 | AAGL |
| ATOM | 869 | OH  | TYR | 111 | 15.104 | 6.183  | 115.423 | 1.00 | 34.00 | AAGL |
| ATOM | 870 | C   | TYR | 111 | 10.505 | 10.246 | 114.832 | 1.00 | 24.33 | AAGL |
| ATOM | 871 | O   | TYR | 111 | 11.307 | 10.383 | 113.901 | 1.00 | 26.25 | AAGL |
| ATOM | 872 | N   | ASN | 112 | 9.398  | 9.521  | 114.731 | 1.00 | 23.20 | AAGL |
| ATOM | 873 | CA  | ASN | 112 | 9.042  | 8.842  | 113.492 | 1.00 | 24.57 | AAGL |
| ATOM | 874 | CB  | ASN | 112 | 7.750  | 8.041  | 113.688 | 1.00 | 27.15 | AAGL |
| ATOM | 875 | CG  | ASN | 112 | 7.963  | 6.757  | 114.473 | 0.50 | 25.91 | AAGL |
| ATOM | 876 | OD1 | ASN | 112 | 7.010  | 6.023  | 114.752 | 0.50 | 29.07 | AAGL |
| ATOM | 877 | ND2 | ASN | 112 | 9.209  | 6.475  | 114.825 | 0.50 | 26.44 | AAGL |
| ATOM | 878 | C   | ASN | 112 | 8.865  | 9.865  | 112.364 | 1.00 | 26.29 | AAGL |
| ATOM | 879 | O   | ASN | 112 | 9.227  | 9.607  | 111.211 | 1.00 | 23.16 | AAGL |
| ATOM | 880 | N   | TYR | 113 | 8.317  | 11.028 | 112.702 | 1.00 | 23.87 | AAGL |
| ATOM | 881 | CA  | TYR | 113 | 8.097  | 12.075 | 111.711 | 1.00 | 23.73 | AAGL |
| ATOM | 882 | CB  | TYR | 113 | 7.328  | 13.239 | 112.315 | 1.00 | 23.08 | AAGL |
| ATOM | 883 | CG  | TYR | 113 | 7.148  | 14.387 | 111.341 | 1.00 | 22.30 | AAGL |
| ATOM | 884 | CD1 | TYR | 113 | 6.290  | 14.271 | 110.243 | 1.00 | 20.43 | AAGL |
| ATOM | 885 | CE1 | TYR | 113 | 6.134  | 15.327 | 109.335 | 1.00 | 21.15 | AAGL |
| ATOM | 886 | CD2 | TYR | 113 | 7.847  | 15.584 | 111.510 | 1.00 | 20.85 | AAGL |
| ATOM | 887 | CE2 | TYR | 113 | 7.699  | 16.642 | 110.612 | 1.00 | 18.32 | AAGL |
| ATOM | 888 | CZ  | TYR | 113 | 6.846  | 16.512 | 109.533 | 1.00 | 19.02 | AAGL |
| ATOM | 889 | OH  | TYR | 113 | 6.706  | 17.562 | 108.654 | 1.00 | 18.05 | AAGL |
| ATOM | 890 | C   | TYR | 113 | 9.391  | 12.613 | 111.111 | 1.00 | 23.40 | AAGL |
| ATOM | 891 | O   | TYR | 113 | 9.561  | 12.611 | 109.891 | 1.00 | 24.13 | AAGL |
| ATOM | 892 | N   | THR | 114 | 10.300 | 13.085 | 111.957 | 1.00 | 22.35 | AAGL |
| ATOM | 893 | CA  | THR | 114 | 11.552 | 13.623 | 111.441 | 1.00 | 23.52 | AAGL |
| ATOM | 894 | CB  | THR | 114 | 12.413 | 14.260 | 112.569 | 1.00 | 22.78 | AAGL |
| ATOM | 895 | OG1 | THR | 114 | 12.714 | 13.292 | 113.578 | 1.00 | 23.02 | AAGL |
| ATOM | 896 | CG2 | THR | 114 | 11.662 | 15.433 | 113.210 | 1.00 | 22.56 | AAGL |
| ATOM | 897 | C   | THR | 114 | 12.339 | 12.530 | 110.711 | 1.00 | 24.38 | AAGL |
| ATOM | 898 | O   | THR | 114 | 12.954 | 12.783 | 109.673 | 1.00 | 23.70 | AAGL |
| ATOM | 899 | N   | LEU | 115 | 12.309 | 11.315 | 111.250 | 1.00 | 26.01 | AAGL |
| ATOM | 900 | CA  | LEU | 115 | 12.995 | 10.189 | 110.618 | 1.00 | 26.48 | AAGL |
| ATOM | 901 | CB  | LEU | 115 | 12.785 | 8.909  | 111.443 | 1.00 | 27.61 | AAGL |
| ATOM | 902 | CG  | LEU | 115 | 13.278 | 7.573  | 110.853 | 1.00 | 28.64 | AAGL |
| ATOM | 903 | CD1 | LEU | 115 | 14.787 | 7.644  | 110.546 | 1.00 | 29.41 | AAGL |
| ATOM | 904 | CD2 | LEU | 115 | 12.991 | 6.434  | 111.836 | 1.00 | 31.02 | AAGL |
| ATOM | 905 | C   | LEU | 115 | 12.432 | 10.002 | 109.208 | 1.00 | 27.33 | AAGL |
| ATOM | 906 | O   | LEU | 115 | 13.180 | 9.902  | 108.236 | 1.00 | 29.69 | AAGL |
| ATOM | 907 | N   | GLU | 116 | 11.106 | 9.979  | 109.102 | 1.00 | 27.14 | AAGL |
| ATOM | 908 | CA  | GLU | 116 | 10.428 | 9.800  | 107.825 | 1.00 | 28.85 | AAGL |
| ATOM | 909 | CB  | GLU | 116 | 8.919  | 9.674  | 108.057 | 1.00 | 33.11 | AAGL |
| ATOM | 910 | CG  | GLU | 116 | 8.111  | 9.374  | 106.803 | 1.00 | 40.59 | AAGL |
| ATOM | 911 | CD  | GLU | 116 | 8.196  | 7.914  | 106.368 | 1.00 | 44.26 | AAGL |
| ATOM | 912 | OE1 | GLU | 116 | 7.696  | 7.603  | 105.266 | 1.00 | 47.23 | AAGL |
| ATOM | 913 | OE2 | GLU | 116 | 8.744  | 7.073  | 107.118 | 1.00 | 47.05 | AAGL |
| ATOM | 914 | C   | GLU | 116 | 10.707 | 10.952 | 106.853 | 1.00 | 28.50 | AAGL |
| ATOM | 915 | O   | GLU | 116 | 10.936 | 10.730 | 105.667 | 1.00 | 28.60 | AAGL |
| ATOM | 916 | N   | VAL | 117 | 10.671 | 12.184 | 107.354 | 1.00 | 25.75 | AAGL |
| ATOM | 917 | CA  | VAL | 117 | 10.933 | 13.345 | 106.507 | 1.00 | 25.01 | AAGL |
| ATOM | 918 | CB  | VAL | 117 | 10.841 | 14.657 | 107.303 | 1.00 | 25.08 | AAGL |
| ATOM | 919 | CG1 | VAL | 117 | 11.393 | 15.810 | 106.473 | 1.00 | 24.84 | AAGL |
| ATOM | 920 | CG2 | VAL | 117 | 9.390  | 14.924 | 107.685 | 1.00 | 25.17 | AAGL |
| ATOM | 921 | C   | VAL | 117 | 12.321 | 13.256 | 105.894 | 1.00 | 25.14 | AAGL |
| ATOM | 922 | O   | VAL | 117 | 12.488 | 13.445 | 104.684 | 1.00 | 26.07 | AAGL |
| ATOM | 923 | N   | CYS | 118 | 13.313 | 12.982 | 106.734 | 1.00 | 22.94 | AAGL |
| ATOM | 924 | CA  | CYS | 118 | 14.684 | 12.868 | 106.261 | 1.00 | 24.56 | AAGL |
| ATOM | 925 | CB  | CYS | 118 | 15.644 | 12.710 | 107.446 | 1.00 | 24.73 | AAGL |
| ATOM | 926 | SG  | CYS | 118 | 15.852 | 14.220 | 108.485 | 1.00 | 26.92 | AAGL |

# Fig. 3 cont.

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| ATOM | 927 | C   | CYS | 118 | 14.810 | 11.682 | 105.289 | 1.00 | 25.33 | AAGL |
|------|-----|-----|-----|-----|--------|--------|---------|------|-------|------|
| ATOM | 928 | O   | CYS | 118 | 15.417 | 11.813 | 104.228 | 1.00 | 25.49 | AAGL |
| ATOM | 929 | N   | ASN | 119 | 14.224 | 10.537 | 105.638 | 1.00 | 25.35 | AAGL |
| ATOM | 930 | CA  | ASN | 119 | 14.296 | 9.372  | 104.753 | 1.00 | 28.13 | AAGL |
| ATOM | 931 | CB  | ASN | 119 | 13.618 | 8.156  | 105.382 | 1.00 | 28.39 | AAGL |
| ATOM | 932 | CG  | ASN | 119 | 14.446 | 7.539  | 106.477 | 1.00 | 28.84 | AAGL |
| ATOM | 933 | OD1 | ASN | 119 | 15.607 | 7.906  | 106.681 | 1.00 | 28.82 | AAGL |
| ATOM | 934 | ND2 | ASN | 119 | 13.858 | 6.592  | 107.191 | 1.00 | 31.56 | AAGL |
| ATOM | 935 | C · | ASN | 119 | 13.685 | 9.618  | 103.381 | 1.00 | 28.08 | AAGL |
| ATOM | 936 | O   | ASN | 119 | 14.199 | 9.129  | 102.376 | 1.00 | 31.49 | AAGL |
| ATOM | 937 | N   | THR | 120 | 12.594 | 10.372 | 103.326 | 1.00 | 28.01 | AAGL |
| ATOM | 938 | CA  | THR | 120 | 11.952 | 10.641 | 102.046 | 1.00 | 27.89 | AAGL |
| ATOM | 939 | CB  | THR | 120 | 10.596 | 11.321 | 102.231 | 1.00 | 30.29 | AAGL |
| ATOM | 940 | OG1 | THR | 120 | 9.752  | 10.480 | 103.034 | 1.00 | 31.43 | AAGL |
| ATOM | 941 | CG2 | THR | 120 | 9.926  | 11.536 | 100.873 | 1.00 | 30.28 | AAGL |
| ATOM | 942 | C   | THR | 120 | 12.838 | 11.495 | 101.147 | 1.00 | 28.78 | AAGL |
| ATOM | 943 | O   | THR | 120 | 12.869 | 11.290 | 99.933  | 1.00 | 29.09 | AAGL |
| ATOM | 944 | N   | PHE | 121 | 13.557 | 12.452 | 101.728 | 1.00 | 28.45 | AAGL |
| ATOM | 945 | CA  | PHE | 121 | 14.463 | 13.269 | 100.930 | 1.00 | 28.19 | AAGL |
| ATOM | 946 | CB  | PHE | 121 | 14.985 | 14.461 | 101.741 | 1.00 | 29.04 | AAGL |
| ATOM | 947 | CG  | PHE | 121 | 14.023 | 15.616 | 101.789 | 1.00 | 27.88 | AAGL |
| ATOM | 948 | CD1 | PHE | 121 | 12.847 | 15.529 | 102.530 | 1.00 | 28.91 | AAGL |
| ATOM | 949 | CD2 | PHE | 121 | 14.242 | 16.753 | 101.018 | 1.00 | 28.77 | AAGL |
| ATOM | 950 | CE1 | PHE | 121 | 11.905 | 16.549 | 102.496 | 1.00 | 26.83 | AAGL |
| ATOM | 951 | CE2 | PHE | 121 | 13.301 | 17.780 | 100.979 | 1.00 | 29.21 | AAGL |
| ATOM | 952 | CZ  | PHE | 121 | 12.130 | 17.676 | 101.719 | 1.00 | 29.40 | AAGL |
| ATOM | 953 | C   | PHE | 121 | 15.622 | 12.391 | 100.454 | 1.00 | 28.62 | AAGL |
| ATOM | 954 | O   | PHE | 121 | 16.064 | 12.485 | 99.308  | 1.00 | 29.15 | AAGL |
| ATOM | 955 | N   | ALA | 122 | 16.102 | 11.519 | 101.332 | 1.00 | 28.34 | AAGL |
| ATOM | 956 | CA  | ALA | 122 | 17.187 | 10.622 | 100.964 | 1.00 | 29.64 | AAGL |
| ATOM | 957 | CB  | ALA | 122 | 17.599 | 9.768  | 102.158 | 1.00 | 27.49 | AAGL |
| ATOM | 958 | C   | ALA | 122 | 16.748 | 9.731  | 99.795  | 1.00 | 29.44 | AAGL |
| ATOM | 959 | O   | ALA | 122 | 17.538 | 9.447  | 98.890  | 1.00 | 30.54 | AAGL |
| ATOM | 960 | N   | GLU | 123 | 15.492 | 9.295  | 99.801  | 1.00 | 27.94 | AAGL |
| ATOM | 961 | CA  | GLU | 123 | 15.004 | 8.448  | 98.720  | 1.00 | 28.60 | AAGL |
| ATOM | 962 | CB  | GLU | 123 | 13.654 | 7.837  | 99.085  | 1.00 | 30.65 | AAGL |
| ATOM | 963 | CG  | GLU | 123 | 13.693 | 7.161  | 100.439 | 1.00 | 35.94 | AAGL |
| ATOM | 964 | CD  | GLU | 123 | 12.401 | 6.467  | 100.813 | 1.00 | 38.73 | AAGL |
| ATOM | 965 | OE1 | GLU | 123 | 11.315 | 6.915  | 100.376 | 1.00 | 39.11 | AAGL |
| ATOM | 966 | OE2 | GLU | 123 | 12.485 | 5.476  | 101.570 | 1.00 | 39.90 | AAGL |
| ATOM | 967 | C   | GLU | 123 | 14.899 | 9.237  | 97.420  | 1.00 | 28.83 | AAGL |
| ATOM | 968 | O   | GLU | 123 | 14.826 | 8.658  | 96.338  | 1.00 | 25.94 | AAGL |
| ATOM | 969 | N   | ASN | 124 | 14.893 | 10.561 | 97.535  | 1.00 | 27.22 | AAGL |
| ATOM | 970 | CA  | ASN | 124 | 14.825 | 11.434 | 96.366  | 1.00 | 26.84 | AAGL |
| ATOM | 971 | CB  | ASN | 124 | 13.786 | 12.537 | 96.579  | 1.00 | 27.25 | AAGL |
| ATOM | 972 | CG  | ASN | 124 | 12.367 | 12.067 | 96.302  | 1.00 | 28.47 | AAGL |
| ATOM | 973 | OD1 | ASN | 124 | 11.888 | 12.130 | 95.168  | 1.00 | 28.23 | AAGL |
| ATOM | 974 | ND2 | ASN | 124 | 11.691 | 11.580 | 97.336  | 1.00 | 30.75 | AAGL |
| ATOM | 975 | C   | ASN | 124 | 16.186 | 12.063 | 96.085  | 1.00 | 26.40 | AAGL |
| ATOM | 976 | O   | ASN | 124 | 16.290 | 13.015 | 95.315  | 1.00 | 25.52 | AAGL |
| ATOM | 977 | N   | ASP | 125 | 17.223 | 11.538 | 96.726  | 1.00 | 26.35 | AAGL |
| ATOM | 978 | CA  | ASP | 125 | 18.580 | 12.039 | 96.532  | 1.00 | 29.66 | AAGL |
| ATOM | 979 | CB  | ASP | 125 | 19.066 | 11.654 | 95.131  | 1.00 | 31.58 | AAGL |
| ATOM | 980 | CG  | ASP | 125 | 20.550 | 11.898 | 94.939  | 1.00 | 34.86 | AAGL |
| ATOM | 981 | OD1 | ASP | 125 | 21.314 | 11.723 | 95.912  | 1.00 | 36.55 | AAGL |
| ATOM | 982 | OD2 | ASP | 125 | 20.958 | 12.254 | 93.813  | 1.00 | 35.76 | AAGL |
| ATOM | 983 | C   | ASP | 125 | 18.715 | 13.555 | 96.738  | 1.00 | 30.52 | AAGL |
| ATOM | 984 | O   | ASP | 125 | 19.286 | 14.265 | 95.906  | 1.00 | 28.80 | AAGL |
| ATOM | 985 | N   | ILE | 126 | 18.181 | 14.042 | 97.853  | 1.00 | 30.01 | AAGL |
| ATOM | 986 | CA  | ILE | 126 | 18.270 | 15.458 | 98.200  | 1.00 | 30.54 | AAGL |
| ATOM | 987 | CB  | ILE | 126 | 16.886 | 16.127 | 98.234  | 1.00 | 30.36 | AAGL |
| ATOM | 988 | CG2 | ILE | 126 | 17.014 | 17.532 | 98.817  | 1.00 | 31.24 | AAGL |
| ATOM | 989 | CG1 | ILE | 126 | 16.294 | 16.182 | 96.823  | 1.00 | 29.46 | AAGL |
| ATOM | 990 | CD1 | ILE | 126 | 14.803 | 16.480 | 96.798  | 1.00 | 32.42 | AAGL |
| ATOM | 991 | C   | ILE | 126 | 18.894 | 15.566 | 99.590  | 1.00 | 32.08 | AAGL |
| ATOM | 992 | O   | ILE | 126 | 18.381 | 14.988 | 100.550 | 1.00 | 33.29 | AAGL |
| ATOM | 993 | N   | ASP | 127 | 20.004 | 16.292 | 99.689  | 1.00 | 30.97 | AAGL |

## Fig. 3 cont.

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| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 994 | CA | ASP | 127 | 20.701 | 16.475 | 100.960 | 1.00 | 32.32 | AAGL |
| ATOM | 995 | CB | ASP | 127 | 22.181 | 16.777 | 100.719 | 1.00 | 36.39 | AAGL |
| ATOM | 996 | CG | ASP | 127 | 22.849 | 15.758 | 99.822 | 1.00 | 40.70 | AAGL |
| ATOM | 997 | OD1 | ASP | 127 | 23.019 | 14.591 | 100.244 | 1.00 | 43.54 | AAGL |
| ATOM | 998 | OD2 | ASP | 127 | 23.201 | 16.126 | 98.680 | 1.00 | 45.38 | AAGL |
| ATOM | 999 | C | ASP | 127 | 20.082 | 17.655 | 101.687 | 1.00 | 31.14 | AAGL |
| ATOM | 1000 | O | ASP | 127 | 19.643 | 18.616 | 101.053 | 1.00 | 30.94 | AAGL |
| ATOM | 1001 | N | ILE | 128 | 20.063 | 17.587 | 103.012 | 1.00 | 29.03 | AAGL |
| ATOM | 1002 | CA | ILE | 128 | 19.505 | 18.659 | 103.825 | 1.00 | 27.70 | AAGL |
| ATOM | 1003 | CB | ILE | 128 | 18.442 | 18.112 | 104.806 | 1.00 | 27.94 | AAGL |
| ATOM | 1004 | CG2 | ILE | 128 | 17.866 | 19.250 | 105.645 | 1.00 | 25.95 | AAGL |
| ATOM | 1005 | CG1 | ILE | 128 | 17.333 | 17.408 | 104.017 | 1.00 | 27.55 | AAGL |
| ATOM | 1006 | CD1 | ILE | 128 | 16.289 | 16.716 | 104.883 | 1.00 | 29.46 | AAGL |
| ATOM | 1007 | C | ILE | 128 | 20.630 | 19.317 | 104.611 | 1.00 | 25.60 | AAGL |
| ATOM | 1008 | O | ILE | 128 | 21.370 | 18.645 | 105.328 | 1.00 | 28.07 | AAGL |
| ATOM | 1009 | N | GLU | 129 | 20.766 | 20.632 | 104.465 | 1.00 | 24.98 | AAGL |
| ATOM | 1010 | CA | GLU | 129 | 21.818 | 21.380 | 105.156 | 1.00 | 24.49 | AAGL |
| ATOM | 1011 | CB | GLU | 129 | 22.107 | 22.671 | 104.382 | 1.00 | 27.35 | AAGL |
| ATOM | 1012 | CG | GLU | 129 | 23.218 | 23.552 | 104.946 | 1.00 | 30.16 | AAGL |
| ATOM | 1013 | CD | GLU | 129 | 24.601 | 22.996 | 104.682 | 1.00 | 32.15 | AAGL |
| ATOM | 1014 | OE1 | GLU | 129 | 24.720 | 22.097 | 103.821 | 1.00 | 32.40 | AAGL |
| ATOM | 1015 | OE2 | GLU | 129 | 25.563 | 23.469 | 105.326 | 1.00 | 31.39 | AAGL |
| ATOM | 1016 | C | GLU | 129 | 21.418 | 21.713 | 106.593 | 1.00 | 24.14 | AAGL |
| ATOM | 1017 | O | GLU | 129 | 22.210 | 21.561 | 107.531 | 1.00 | 23.23 | AAGL |
| ATOM | 1018 | N | ILE | 130 | 20.184 | 22.174 | 106.761 | 1.00 | 22.11 | AAGL |
| ATOM | 1019 | CA | ILE | 130 | 19.696 | 22.535 | 108.083 | 1.00 | 20.15 | AAGL |
| ATOM | 1020 | CB | ILE | 130 | 19.719 | 24.065 | 108.301 | 1.00 | 21.07 | AAGL |
| ATOM | 1021 | CG2 | ILE | 130 | 19.096 | 24.406 | 109.636 | 1.00 | 22.31 | AAGL |
| ATOM | 1022 | CG1 | ILE | 130 | 21.147 | 24.601 | 108.233 | 1.00 | 20.04 | AAGL |
| ATOM | 1023 | CD1 | ILE | 130 | 21.215 | 26.109 | 108.266 | 1.00 | 21.74 | AAGL |
| ATOM | 1024 | C | ILE | 130 | 18.256 | 22.091 | 108.265 | 1.00 | 20.32 | AAGL |
| ATOM | 1025 | O | ILE | 130 | 17.464 | 22.096 | 107.328 | 1.00 | 18.94 | AAGL |
| ATOM | 1026 | N | ILE | 131 | 17.920 | 21.696 | 109.480 | 1.00 | 21.44 | AAGL |
| ATOM | 1027 | CA | ILE | 131 | 16.551 | 21.316 | 109.759 | 1.00 | 22.36 | AAGL |
| ATOM | 1028 | CB | ILE | 131 | 16.324 | 19.791 | 109.544 | 1.00 | 23.90 | AAGL |
| ATOM | 1029 | CG2 | ILE | 131 | 17.138 | 18.979 | 110.541 | 1.00 | 28.54 | AAGL |
| ATOM | 1030 | CG1 | ILE | 131 | 14.826 | 19.488 | 109.629 | 1.00 | 26.48 | AAGL |
| ATOM | 1031 | CD1 | ILE | 131 | 14.427 | 18.156 | 109.005 | 1.00 | 28.03 | AAGL |
| ATOM | 1032 | C | ILE | 131 | 16.253 | 21.765 | 111.185 | 1.00 | 21.53 | AAGL |
| ATOM | 1033 | O | ILE | 131 | 16.978 | 21.430 | 112.119 | 1.00 | 20.84 | AAGL |
| ATOM | 1034 | N | SER | 132 | 15.217 | 22.587 | 111.335 | 1.00 | 20.93 | AAGL |
| ATOM | 1035 | CA | SER | 132 | 14.859 | 23.089 | 112.654 | 1.00 | 19.31 | AAGL |
| ATOM | 1036 | CB | SER | 132 | 14.444 | 24.562 | 112.578 | 1.00 | 18.01 | AAGL |
| ATOM | 1037 | OG | SER | 132 | 13.232 | 24.709 | 111.869 | 1.00 | 21.72 | AAGL |
| ATOM | 1038 | C | SER | 132 | 13.720 | 22.261 | 113.221 | 1.00 | 19.27 | AAGL |
| ATOM | 1039 | O | SER | 132 | 12.766 | 21.930 | 112.520 | 1.00 | 19.32 | AAGL |
| ATOM | 1040 | N | ILE | 133 | 13.842 | 21.901 | 114.491 | 1.00 | 19.77 | AAGL |
| ATOM | 1041 | CA | ILE | 133 | 12.806 | 21.122 | 115.143 | 1.00 | 20.58 | AAGL |
| ATOM | 1042 | CB | ILE | 133 | 13.367 | 20.295 | 116.317 | 1.00 | 21.64 | AAGL |
| ATOM | 1043 | CG2 | ILE | 133 | 12.297 | 19.334 | 116.823 | 1.00 | 18.97 | AAGL |
| ATOM | 1044 | CG1 | ILE | 133 | 14.644 | 19.559 | 115.890 | 1.00 | 21.37 | AAGL |
| ATOM | 1045 | CD1 | ILE | 133 | 14.515 | 18.774 | 114.605 | 1.00 | 25.39 | AAGL |
| ATOM | 1046 | C | ILE | 133 | 11.815 | 22.142 | 115.689 | 1.00 | 20.75 | AAGL |
| ATOM | 1047 | O | ILE | 133 | 11.890 | 22.529 | 116.850 | 1.00 | 21.44 | AAGL |
| ATOM | 1048 | N | GLY | 134 | 10.904 | 22.581 | 114.833 | 1.00 | 19.14 | AAGL |
| ATOM | 1049 | CA | GLY | 134 | 9.919 | 23.560 | 115.241 | 1.00 | 18.88 | AAGL |
| ATOM | 1050 | C | GLY | 134 | 10.240 | 24.936 | 114.690 | 1.00 | 18.31 | AAGL |
| ATOM | 1051 | O | GLY | 134 | 11.344 | 25.181 | 114.199 | 1.00 | 19.16 | AAGL |
| ATOM | 1052 | N | ASN | 135 | 9.268 | 25.835 | 114.769 | 1.00 | 16.66 | AAGL |
| ATOM | 1053 | CA | ASN | 135 | 9.427 | 27.201 | 114.289 | 1.00 | 16.54 | AAGL |
| ATOM | 1054 | CB | ASN | 135 | 8.507 | 27.457 | 113.097 | 1.00 | 15.67 | AAGL |
| ATOM | 1055 | CG | ASN | 135 | 8.666 | 28.854 | 112.532 | 1.00 | 20.06 | AAGL |
| ATOM | 1056 | OD1 | ASN | 135 | 9.590 | 29.120 | 111.759 | 1.00 | 19.47 | AAGL |
| ATOM | 1057 | ND2 | ASN | 135 | 7.773 | 29.762 | 112.932 | 1.00 | 14.55 | AAGL |
| ATOM | 1058 | C | ASN | 135 | 9.044 | 28.146 | 115.420 | 1.00 | 17.93 | AAGL |
| ATOM | 1059 | O | ASN | 135 | 7.940 | 28.063 | 115.935 | 1.00 | 16.64 | AAGL |
| ATOM | 1060 | N | GLU | 136 | 9.967 | 29.030 | 115.793 | 1.00 | 16.85 | AAGL |

# Fig. 3 cont.

| ATOM | 1061 | CA | GLU | 136 | 9.760 | 30.001 | 116.865 | 1.00 | 17.43 | AAGL |
|------|------|----|----|-----|-------|--------|---------|------|-------|------|
| ATOM | 1062 | CB | GLU | 136 | 8.892 | 31.169 | 116.371 | 1.00 | 18.10 | AAGL |
| ATOM | 1063 | CG | GLU | 136 | 9.517 | 31.970 | 115.228 | 1.00 | 17.17 | AAGL |
| ATOM | 1064 | CD | GLU | 136 | 8.747 | 33.240 | 114.867 | 1.00 | 18.85 | AAGL |
| ATOM | 1065 | OE1 | GLU | 136 | 7.592 | 33.416 | 115.314 | 1.00 | 19.27 | AAGL |
| ATOM | 1066 | OE2 | GLU | 136 | 9.305 | 34.071 | 114.120 | 1.00 | 18.05 | AAGL |
| ATOM | 1067 | C | GLU | 136 | 9.116 | 29.338 | 118.080 | 1.00 | 17.00 | AAGL |
| ATOM | 1068 | O | GLU | 136 | 8.013 | 29.697 | 118.478 | 1.00 | 18.88 | AAGL |
| ATOM | 1069 | N | ILE | 137 | 9.819 | 28.379 | 118.674 | 1.00 | 16.48 | AAGL |
| ATOM | 1070 | CA | ILE | 137 | 9.283 | 27.657 | 119.828 | 1.00 | 16.33 | AAGL |
| ATOM | 1071 | CB | ILE | 137 | 9.753 | 26.185 | 119.830 | 1.00 | 17.11 | AAGL |
| ATOM | 1072 | CG2 | ILE | 137 | 9.204 | 25.457 | 118.615 | 1.00 | 18.25 | AAGL |
| ATOM | 1073 | CG1 | ILE | 137 | 11.276 | 26.119 | 119.848 | 1.00 | 18.08 | AAGL |
| ATOM | 1074 | CD1 | ILE | 137 | 11.822 | 24.717 | 120.029 | 1.00 | 19.03 | AAGL |
| ATOM | 1075 | C | ILE | 137 | 9.600 | 28.266 | 121.200 | 1.00 | 16.65 | AAGL |
| ATOM | 1076 | O | ILE | 137 | 9.770 | 27.540 | 122.178 | 1.00 | 18.23 | AAGL |
| ATOM | 1077 | N | ARG | 138 | 9.668 | 29.591 | 121.271 | 1.00 | 15.75 | AAGL |
| ATOM | 1078 | CA | ARG | 138 | 9.948 | 30.265 | 122.537 | 1.00 | 19.97 | AAGL |
| ATOM | 1079 | CB | ARG | 138 | 10.069 | 31.776 | 122.327 | 1.00 | 21.48 | AAGL |
| ATOM | 1080 | CG | ARG | 138 | 10.434 | 32.559 | 123.586 | 1.00 | 23.19 | AAGL |
| ATOM | 1081 | CD | ARG | 138 | 10.971 | 33.946 | 123.230 | 1.00 | 25.82 | AAGL |
| ATOM | 1082 | NE | ARG | 138 | 10.007 | 34.726 | 122.454 | 1.00 | 29.47 | AAGL |
| ATOM | 1083 | CZ | ARG | 138 | 8.900 | 35.263 | 122.956 | 1.00 | 29.69 | AAGL |
| ATOM | 1084 | NH1 | ARG | 138 | 8.610 | 35.110 | 124.243 | 1.00 | 32.98 | AAGL |
| ATOM | 1085 | NH2 | ARG | 138 | 8.075 | 35.939 | 122.168 | 1.00 | 29.53 | AAGL |
| ATOM | 1086 | C | ARG | 138 | 8.852 | 29.971 | 123.557 | 1.00 | 20.72 | AAGL |
| ATOM | 1087 | O | ARG | 138 | 9.112 | 29.926 | 124.755 | 1.00 | 22.83 | AAGL |
| ATOM | 1088 | N | ALA | 139 | 7.624 | 29.788 | 123.081 | 1.00 | 19.30 | AAGL |
| ATOM | 1089 | CA | ALA | 139 | 6.513 | 29.470 | 123.969 | 1.00 | 19.27 | AAGL |
| ATOM | 1090 | CB | ALA | 139 | 5.268 | 30.275 | 123.586 | 1.00 | 21.29 | AAGL |
| ATOM | 1091 | C | ALA | 139 | 6.227 | 27.971 | 123.893 | 1.00 | 20.13 | AAGL |
| ATOM | 1092 | O | ALA | 139 | 5.102 | 27.517 | 124.135 | 1.00 | 19.76 | AAGL |
| ATOM | 1093 | N | GLY | 140 | 7.264 | 27.207 | 123.565 | 1.00 | 16.96 | AAGL |
| ATOM | 1094 | CA | GLY | 140 | 7.124 | 25.769 | 123.465 | 1.00 | 17.78 | AAGL |
| ATOM | 1095 | C | GLY | 140 | 6.640 | 25.305 | 122.102 | 1.00 | 18.69 | AAGL |
| ATOM | 1096 | O | GLY | 140 | 6.669 | 26.058 | 121.119 | 1.00 | 15.87 | AAGL |
| ATOM | 1097 | N | LEU | 141 | 6.185 | 24.058 | 122.051 | 1.00 | 18.79 | AAGL |
| ATOM | 1098 | CA | LEU | 141 | 5.689 | 23.458 | 120.815 | 1.00 | 18.06 | AAGL |
| ATOM | 1099 | CB | LEU | 141 | 6.855 | 22.900 | 119.999 | 1.00 | 17.19 | AAGL |
| ATOM | 1100 | CG | LEU | 141 | 7.477 | 21.595 | 120.523 | 1.00 | 18.49 | AAGL |
| ATOM | 1101 | CD1 | LEU | 141 | 8.404 | 21.018 | 119.457 | 1.00 | 17.04 | AAGL |
| ATOM | 1102 | CD2 | LEU | 141 | 8.231 | 21.842 | 121.827 | 1.00 | 17.24 | AAGL |
| ATOM | 1103 | C | LEU | 141 | 4.741 | 22.310 | 121.145 | 1.00 | 17.11 | AAGL |
| ATOM | 1104 | O | LEU | 141 | 4.632 | 21.901 | 122.295 | 1.00 | 19.24 | AAGL |
| ATOM | 1105 | N | LEU | 142 | 4.063 | 21.795 | 120.126 | 1.00 | 15.85 | AAGL |
| ATOM | 1106 | CA | LEU | 142 | 3.162 | 20.664 | 120.293 | 1.00 | 16.79 | AAGL |
| ATOM | 1107 | CB | LEU | 142 | 3.981 | 19.370 | 120.301 | 1.00 | 17.91 | AAGL |
| ATOM | 1108 | CG | LEU | 142 | 4.783 | 19.127 | 119.017 | 1.00 | 18.45 | AAGL |
| ATOM | 1109 | CD1 | LEU | 142 | 5.725 | 17.947 | 119.195 | 1.00 | 16.19 | AAGL |
| ATOM | 1110 | CD2 | LEU | 142 | 3.827 | 18.888 | 117.861 | 1.00 | 18.62 | AAGL |
| ATOM | 1111 | C | LEU | 142 | 2.319 | 20.766 | 121.562 | 1.00 | 18.08 | AAGL |
| ATOM | 1112 | O | LEU | 142 | 2.374 | 19.909 | 122.440 | 1.00 | 18.47 | AAGL |
| ATOM | 1113 | N | TRP | 143 | 1.539 | 21.830 | 121.652 | 1.00 | 18.54 | AAGL |
| ATOM | 1114 | CA | TRP | 143 | 0.684 | 22.038 | 122.810 | 1.00 | 18.96 | AAGL |
| ATOM | 1115 | CB | TRP | 143 | 0.063 | 23.431 | 122.763 | 1.00 | 17.05 | AAGL |
| ATOM | 1116 | CG | TRP | 143 | 1.061 | 24.544 | 122.780 | 1.00 | 15.57 | AAGL |
| ATOM | 1117 | CD2 | TRP | 143 | 0.807 | 25.920 | 122.475 | 1.00 | 16.04 | AAGL |
| ATOM | 1118 | CE2 | TRP | 143 | 2.014 | 26.621 | 122.675 | 1.00 | 15.69 | AAGL |
| ATOM | 1119 | CE3 | TRP | 143 | -0.324 | 26.629 | 122.053 | 1.00 | 17.45 | AAGL |
| ATOM | 1120 | CD1 | TRP | 143 | 2.375 | 24.468 | 123.139 | 1.00 | 15.44 | AAGL |
| ATOM | 1121 | NE1 | TRP | 143 | 2.954 | 25.711 | 123.081 | 1.00 | 14.73 | AAGL |
| ATOM | 1122 | CZ2 | TRP | 143 | 2.120 | 27.998 | 122.467 | 1.00 | 18.72 | AAGL |
| ATOM | 1123 | CZ3 | TRP | 143 | -0.215 | 28.000 | 121.848 | 1.00 | 20.29 | AAGL |
| ATOM | 1124 | CH2 | TRP | 143 | 0.995 | 28.666 | 122.055 | 1.00 | 18.09 | AAGL |
| ATOM | 1125 | C | TRP | 143 | -0.420 | 20.989 | 122.830 | 1.00 | 17.60 | AAGL |
| ATOM | 1126 | O | TRP | 143 | -0.860 | 20.526 | 121.787 | 1.00 | 19.46 | AAGL |
| ATOM | 1127 | N | PRO | 144 | -0.928 | 20.646 | 124.022 | 1.00 | 19.35 | AAGL |

# Fig. 3 cont.

| | | | | | | | | | | |
|------|------|-----|-----|-----|---------|---------|---------|------|-------|------|
| ATOM | 1128 | CD  | PRO | 144 | -2.116  | 19.777  | 124.132 | 1.00 | 18.54 | AAGL |
| ATOM | 1129 | CA  | PRO | 144 | -0.549  | 21.167  | 125.340 | 1.00 | 18.49 | AAGL |
| ATOM | 1130 | CB  | PRO | 144 | -1.796  | 20.898  | 126.169 | 1.00 | 18.97 | AAGL |
| ATOM | 1131 | CG  | PRO | 144 | -2.228  | 19.560  | 125.628 | 1.00 | 20.05 | AAGL |
| ATOM | 1132 | C   | PRO | 144 | 0.687   | 20.546  | 125.990 | 1.00 | 17.18 | AAGL |
| ATOM | 1133 | O   | PRO | 144 | 1.303   | 21.162  | 126.855 | 1.00 | 17.80 | AAGL |
| ATOM | 1134 | N   | LEU | 145 | 1.043   | 19.329  | 125.592 | 1.00 | 16.38 | AAGL |
| ATOM | 1135 | CA  | LEU | 145 | 2.184   | 18.655  | 126.206 | 1.00 | 18.03 | AAGL |
| ATOM | 1136 | CB  | LEU | 145 | 2.401   | 17.277  | 125.567 | 1.00 | 19.70 | AAGL |
| ATOM | 1137 | CG  | LEU | 145 | 1.382   | 16.208  | 125.988 | 1.00 | 21.47 | AAGL |
| ATOM | 1138 | CD1 | LEU | 145 | 1.529   | 14.966  | 125.133 | 1.00 | 24.17 | AAGL |
| ATOM | 1139 | CD2 | LEU | 145 | 1.584   | 15.871  | 127.450 | 1.00 | 22.76 | AAGL |
| ATOM | 1140 | C   | LEU | 145 | 3.482   | 19.449  | 126.189 | 1.00 | 18.55 | AAGL |
| ATOM | 1141 | O   | LEU | 145 | 4.291   | 19.335  | 127.113 | 1.00 | 18.42 | AAGL |
| ATOM | 1142 | N   | GLY | 146 | 3.671   | 20.262  | 125.152 | 1.00 | 18.88 | AAGL |
| ATOM | 1143 | CA  | GLY | 146 | 4.884   | 21.050  | 125.045 | 1.00 | 18.53 | AAGL |
| ATOM | 1144 | C   | GLY | 146 | 4.759   | 22.511  | 125.444 | 1.00 | 19.09 | AAGL |
| ATOM | 1145 | O   | GLY | 146 | 5.509   | 23.351  | 124.948 | 1.00 | 17.40 | AAGL |
| ATOM | 1146 | N   | GLU | 147 | 3.811   | 22.827  | 126.326 | 1.00 | 18.92 | AAGL |
| ATOM | 1147 | CA  | GLU | 147 | 3.647   | 24.207  | 126.792 | 1.00 | 18.48 | AAGL |
| ATOM | 1148 | CB  | GLU | 147 | 2.298   | 24.382  | 127.499 | 1.00 | 17.73 | AAGL |
| ATOM | 1149 | CG  | GLU | 147 | 1.111   | 24.296  | 126.565 | 1.00 | 18.17 | AAGL |
| ATOM | 1150 | CD  | GLU | 147 | 0.452   | 25.642  | 126.328 | 1.00 | 21.87 | AAGL |
| ATOM | 1151 | OE1 | GLU | 147 | 1.137   | 26.684  | 126.464 | 1.00 | 24.40 | AAGL |
| ATOM | 1152 | OE2 | GLU | 147 | -0.751  | 25.655  | 125.997 | 1.00 | 22.11 | AAGL |
| ATOM | 1153 | C   | GLU | 147 | 4.789   | 24.512  | 127.759 | 1.00 | 19.00 | AAGL |
| ATOM | 1154 | O   | GLU | 147 | 5.421   | 23.589  | 128.287 | 1.00 | 20.89 | AAGL |
| ATOM | 1155 | N   | THR | 148 | 5.046   | 25.797  | 128.003 | 1.00 | 18.85 | AAGL |
| ATOM | 1156 | CA  | THR | 148 | 6.137   | 26.194  | 128.887 | 1.00 | 21.19 | AAGL |
| ATOM | 1157 | CB  | THR | 148 | 6.486   | 27.705  | 128.746 | 1.00 | 21.41 | AAGL |
| ATOM | 1158 | OG1 | THR | 148 | 5.307   | 28.498  | 128.908 | 1.00 | 23.59 | AAGL |
| ATOM | 1159 | CG2 | THR | 148 | 7.095   | 27.987  | 127.379 | 1.00 | 21.18 | AAGL |
| ATOM | 1160 | C   | THR | 148 | 5.889   | 25.868  | 130.354 | 1.00 | 21.42 | AAGL |
| ATOM | 1161 | O   | THR | 148 | 6.711   | 26.180  | 131.207 | 1.00 | 21.58 | AAGL |
| ATOM | 1162 | N   | SER | 149 | 4.753   | 25.251  | 130.656 | 1.00 | 20.92 | AAGL |
| ATOM | 1163 | CA  | SER | 149 | 4.487   | 24.852  | 132.027 | 1.00 | 22.49 | AAGL |
| ATOM | 1164 | CB  | SER | 149 | 2.990   | 24.593  | 132.228 | 1.00 | 20.24 | AAGL |
| ATOM | 1165 | OG  | SER | 149 | 2.442   | 23.871  | 131.142 | 1.00 | 21.26 | AAGL |
| ATOM | 1166 | C   | SER | 149 | 5.314   | 23.582  | 132.275 | 1.00 | 23.11 | AAGL |
| ATOM | 1167 | O   | SER | 149 | 5.420   | 23.093  | 133.397 | 1.00 | 23.52 | AAGL |
| ATOM | 1168 | N   | SER | 150 | 5.914   | 23.062  | 131.205 | 1.00 | 22.32 | AAGL |
| ATOM | 1169 | CA  | SER | 150 | 6.749   | 21.868  | 131.299 | 1.00 | 22.70 | AAGL |
| ATOM | 1170 | CB  | SER | 150 | 5.925   | 20.609  | 131.003 | 1.00 | 23.28 | AAGL |
| ATOM | 1171 | OG  | SER | 150 | 6.735   | 19.445  | 131.058 | 1.00 | 24.36 | AAGL |
| ATOM | 1172 | C   | SER | 150 | 7.946   | 21.937  | 130.345 | 1.00 | 22.43 | AAGL |
| ATOM | 1173 | O   | SER | 150 | 7.909   | 21.386  | 129.246 | 1.00 | 22.55 | AAGL |
| ATOM | 1174 | N   | TYR | 151 | 9.007   | 22.619  | 130.766 | 1.00 | 22.50 | AAGL |
| ATOM | 1175 | CA  | TYR | 151 | 10.195  | 22.714  | 129.932 | 1.00 | 23.76 | AAGL |
| ATOM | 1176 | CB  | TYR | 151 | 11.192  | 23.730  | 130.511 | 1.00 | 23.66 | AAGL |
| ATOM | 1177 | CG  | TYR | 151 | 10.861  | 25.169  | 130.153 | 1.00 | 25.07 | AAGL |
| ATOM | 1178 | CD1 | TYR | 151 | 10.054  | 25.950  | 130.978 | 1.00 | 22.33 | AAGL |
| ATOM | 1179 | CE1 | TYR | 151 | 9.719   | 27.270  | 130.628 | 1.00 | 22.71 | AAGL |
| ATOM | 1180 | CD2 | TYR | 151 | 11.329  | 25.740  | 128.965 | 1.00 | 24.38 | AAGL |
| ATOM | 1181 | CE2 | TYR | 151 | 10.997  | 27.057  | 128.610 | 1.00 | 23.11 | AAGL |
| ATOM | 1182 | CZ  | TYR | 151 | 10.195  | 27.812  | 129.446 | 1.00 | 22.47 | AAGL |
| ATOM | 1183 | OH  | TYR | 151 | 9.881   | 29.113  | 129.116 | 1.00 | 23.02 | AAGL |
| ATOM | 1184 | C   | TYR | 151 | 10.827  | 21.327  | 129.804 | 1.00 | 24.63 | AAGL |
| ATOM | 1185 | O   | TYR | 151 | 11.627  | 21.070  | 128.903 | 1.00 | 23.36 | AAGL |
| ATOM | 1186 | N   | SER | 152 | 10.441  | 20.427  | 130.703 | 1.00 | 25.50 | AAGL |
| ATOM | 1187 | CA  | SER | 152 | 10.942  | 19.064  | 130.670 | 1.00 | 24.95 | AAGL |
| ATOM | 1188 | CB  | SER | 152 | 10.539  | 18.325  | 131.945 | 1.00 | 25.80 | AAGL |
| ATOM | 1189 | OG  | SER | 152 | 11.051  | 17.010  | 131.928 | 1.00 | 31.90 | AAGL |
| ATOM | 1190 | C   | SER | 152 | 10.364  | 18.358  | 129.442 | 1.00 | 23.88 | AAGL |
| ATOM | 1191 | O   | SER | 152 | 11.081  | 17.695  | 128.696 | 1.00 | 24.71 | AAGL |
| ATOM | 1192 | N   | ASN | 153 | 9.059   | 18.502  | 129.229 | 1.00 | 24.00 | AAGL |
| ATOM | 1193 | CA  | ASN | 153 | 8.414   | 17.885  | 128.075 | 1.00 | 22.02 | AAGL |
| ATOM | 1194 | CB  | ASN | 153 | 6.901   | 18.108  | 128.132 | 1.00 | 21.03 | AAGL |

# Fig. 3 cont.

| ATOM | 1195 | CG | ASN | 153 | 6.225 | 17.239 | 129.168 | 1.00 | 22.68 | AAGL |
|------|------|-----|-----|-----|-------|--------|---------|------|-------|------|
| ATOM | 1196 | OD1 | ASN | 153 | 6.888 | 16.579 | 129.971 | 1.00 | 21.72 | AAGL |
| ATOM | 1197 | ND2 | ASN | 153 | 4.897 | 17.235 | 129.159 | 1.00 | 19.51 | AAGL |
| ATOM | 1198 | C | ASN | 153 | 8.970 | 18.486 | 126.782 | 1.00 | 21.57 | AAGL |
| ATOM | 1199 | O | ASN | 153 | 9.178 | 17.782 | 125.792 | 1.00 | 19.66 | AAGL |
| ATOM | 1200 | N | ILE | 154 | 9.192 | 19.797 | 126.798 | 1.00 | 20.58 | AAGL |
| ATOM | 1201 | CA | ILE | 154 | 9.733 | 20.490 | 125.636 | 1.00 | 21.12 | AAGL |
| ATOM | 1202 | CB | ILE | 154 | 9.922 | 21.988 | 125.909 | 1.00 | 21.27 | AAGL |
| ATOM | 1203 | CG2 | ILE | 154 | 10.721 | 22.626 | 124.771 | 1.00 | 20.30 | AAGL |
| ATOM | 1204 | CG1 | ILE | 154 | 8.563 | 22.666 | 126.092 | 1.00 | 20.35 | AAGL |
| ATOM | 1205 | CD1 | ILE | 154 | 8.664 | 24.125 | 126.509 | 1.00 | 21.33 | AAGL |
| ATOM | 1206 | C | ILE | 154 | 11.097 | 19.901 | 125.304 | 1.00 | 22.17 | AAGL |
| ATOM | 1207 | O | ILE | 154 | 11.395 | 19.610 | 124.147 | 1.00 | 19.83 | AAGL |
| ATOM | 1208 | N | GLY | 155 | 11.920 | 19.735 | 126.337 | 1.00 | 23.65 | AAGL |
| ATOM | 1209 | CA | GLY | 155 | 13.246 | 19.181 | 126.147 | 1.00 | 24.02 | AAGL |
| ATOM | 1210 | C | GLY | 155 | 13.201 | 17.756 | 125.635 | 1.00 | 23.51 | AAGL |
| ATOM | 1211 | O | GLY | 155 | 13.968 | 17.384 | 124.745 | 1.00 | 23.80 | AAGL |
| ATOM | 1212 | N | ALA | 156 | 12.300 | 16.952 | 126.191 | 1.00 | 24.34 | AAGL |
| ATOM | 1213 | CA | ALA | 156 | 12.169 | 15.560 | 125.774 | 1.00 | 23.36 | AAGL |
| ATOM | 1214 | CB | ALA | 156 | 11.203 | 14.826 | 126.700 | 1.00 | 25.00 | AAGL |
| ATOM | 1215 | C | ALA | 156 | 11.701 | 15.457 | 124.324 | 1.00 | 23.25 | AAGL |
| ATOM | 1216 | O | ALA | 156 | 12.121 | 14.571 | 123.589 | 1.00 | 22.33 | AAGL |
| ATOM | 1217 | N | LEU | 157 | 10.831 | 16.371 | 123.911 | 1.00 | 22.39 | AAGL |
| ATOM | 1218 | CA | LEU | 157 | 10.340 | 16.376 | 122.538 | 1.00 | 21.31 | AAGL |
| ATOM | 1219 | CB | LEU | 157 | 9.161 | 17.343 | 122.408 | 1.00 | 20.00 | AAGL |
| ATOM | 1220 | CG | LEU | 157 | 7.868 | 16.843 | 123.059 | 1.00 | 22.93 | AAGL |
| ATOM | 1221 | CD1 | LEU | 157 | 6.894 | 17.994 | 123.274 | 1.00 | 22.57 | AAGL |
| ATOM | 1222 | CD2 | LEU | 157 | 7.260 | 15.751 | 122.164 | 1.00 | 21.07 | AAGL |
| ATOM | 1223 | C | LEU | 157 | 11.443 | 16.772 | 121.564 | 1.00 | 21.89 | AAGL |
| ATOM | 1224 | O | LEU | 157 | 11.616 | 16.146 | 120.518 | 1.00 | 20.81 | AAGL |
| ATOM | 1225 | N | LEU | 158 | 12.195 | 17.813 | 121.905 | 1.00 | 21.14 | AAGL |
| ATOM | 1226 | CA | LEU | 158 | 13.267 | 18.257 | 121.021 | 1.00 | 22.43 | AAGL |
| ATOM | 1227 | CB | LEU | 158 | 13.903 | 19.540 | 121.569 | 1.00 | 22.22 | AAGL |
| ATOM | 1228 | CG | LEU | 158 | 12.982 | 20.775 | 121.562 | 1.00 | 21.62 | AAGL |
| ATOM | 1229 | CD1 | LEU | 158 | 13.640 | 21.917 | 122.316 | 1.00 | 21.34 | AAGL |
| ATOM | 1230 | CD2 | LEU | 158 | 12.683 | 21.193 | 120.131 | 1.00 | 21.57 | AAGL |
| ATOM | 1231 | C | LEU | 158 | 14.299 | 17.133 | 120.880 | 1.00 | 24.78 | AAGL |
| ATOM | 1232 | O | LEU | 158 | 14.807 | 16.880 | 119.794 | 1.00 | 23.68 | AAGL |
| ATOM | 1233 | N | HIS | 159 | 14.584 | 16.457 | 121.990 | 1.00 | 24.81 | AAGL |
| ATOM | 1234 | CA | HIS | 159 | 15.518 | 15.332 | 122.009 | 1.00 | 26.46 | AAGL |
| ATOM | 1235 | CB | HIS | 159 | 15.566 | 14.738 | 123.423 | 1.00 | 27.84 | AAGL |
| ATOM | 1236 | CG | HIS | 159 | 16.473 | 13.553 | 123.563 | 1.00 | 30.73 | AAGL |
| ATOM | 1237 | CD2 | HIS | 159 | 16.204 | 12.248 | 123.812 | 1.00 | 32.59 | AAGL |
| ATOM | 1238 | ND1 | HIS | 159 | 17.845 | 13.651 | 123.482 | 1.00 | 31.02 | AAGL |
| ATOM | 1239 | CE1 | HIS | 159 | 18.383 | 12.460 | 123.676 | 1.00 | 32.44 | AAGL |
| ATOM | 1240 | NE2 | HIS | 159 | 17.409 | 11.592 | 123.880 | 1.00 | 33.23 | AAGL |
| ATOM | 1241 | C | HIS | 159 | 15.029 | 14.270 | 121.017 | 1.00 | 26.31 | AAGL |
| ATOM | 1242 | O | HIS | 159 | 15.796 | 13.772 | 120.190 | 1.00 | 26.14 | AAGL |
| ATOM | 1243 | N | SER | 160 | 13.749 | 13.922 | 121.110 | 1.00 | 25.57 | AAGL |
| ATOM | 1244 | CA | SER | 160 | 13.149 | 12.927 | 120.220 | 1.00 | 26.09 | AAGL |
| ATOM | 1245 | CB | SER | 160 | 11.679 | 12.695 | 120.590 | 1.00 | 26.91 | AAGL |
| ATOM | 1246 | OG | SER | 160 | 11.555 | 12.082 | 121.857 | 1.00 | 28.98 | AAGL |
| ATOM | 1247 | C | SER | 160 | 13.225 | 13.333 | 118.745 | 1.00 | 25.22 | AAGL |
| ATOM | 1248 | O | SER | 160 | 13.564 | 12.516 | 117.885 | 1.00 | 26.49 | AAGL |
| ATOM | 1249 | N | GLY | 161 | 12.890 | 14.586 | 118.452 | 1.00 | 22.94 | AAGL |
| ATOM | 1250 | CA | GLY | 161 | 12.934 | 15.051 | 117.078 | 1.00 | 22.94 | AAGL |
| ATOM | 1251 | C | GLY | 161 | 14.359 | 15.017 | 116.556 | 1.00 | 23.15 | AAGL |
| ATOM | 1252 | O | GLY | 161 | 14.631 | 14.541 | 115.450 | 1.00 | 23.15 | AAGL |
| ATOM | 1253 | N | ALA | 162 | 15.277 | 15.519 | 117.368 | 1.00 | 24.30 | AAGL |
| ATOM | 1254 | CA | ALA | 162 | 16.683 | 15.548 | 117.002 | 1.00 | 26.37 | AAGL |
| ATOM | 1255 | CB | ALA | 162 | 17.510 | 16.073 | 118.164 | 1.00 | 24.96 | AAGL |
| ATOM | 1256 | C | ALA | 162 | 17.172 | 14.160 | 116.598 | 1.00 | 27.69 | AAGL |
| ATOM | 1257 | O | ALA | 162 | 17.801 | 13.995 | 115.546 | 1.00 | 27.54 | AAGL |
| ATOM | 1258 | N | TRP | 163 | 16.876 | 13.159 | 117.423 | 1.00 | 27.38 | AAGL |
| ATOM | 1259 | CA | TRP | 163 | 17.320 | 11.806 | 117.124 | 1.00 | 26.93 | AAGL |
| ATOM | 1260 | CB | TRP | 163 | 17.222 | 10.929 | 118.368 | 1.00 | 28.85 | AAGL |
| ATOM | 1261 | CG | TRP | 163 | 18.386 | 11.181 | 119.245 | 1.00 | 31.71 | AAGL |

## Fig. 3 cont.

| ATOM | 1262 | CD2 | TRP | 163 | 19.668 | 10.565 | 119.134 | 1.00 | 32.43 | AAGL |
|------|------|-----|-----|-----|--------|--------|---------|------|-------|------|
| ATOM | 1263 | CE2 | TRP | 163 | 20.516 | 11.194 | 120.068 | 1.00 | 31.66 | AAGL |
| ATOM | 1264 | CE3 | TRP | 163 | 20.185 | 9.541 | 118.329 | 1.00 | 32.40 | AAGL |
| ATOM | 1265 | CD1 | TRP | 163 | 18.497 | 12.130 | 120.217 | 1.00 | 31.49 | AAGL |
| ATOM | 1266 | NE1 | TRP | 163 | 19.776 | 12.149 | 120.715 | 1.00 | 32.86 | AAGL |
| ATOM | 1267 | CZ2 | TRP | 163 | 21.858 | 10.836 | 120.223 | 1.00 | 32.68 | AAGL |
| ATOM | 1268 | CZ3 | TRP | 163 | 21.522 | 9.184 | 118.479 | 1.00 | 32.50 | AAGL |
| ATOM | 1269 | CH2 | TRP | 163 | 22.342 | 9.832 | 119.421 | 1.00 | 32.64 | AAGL |
| ATOM | 1270 | C | TRP | 163 | 16.636 | 11.144 | 115.952 | 1.00 | 27.25 | AAGL |
| ATOM | 1271 | O | TRP | 163 | 17.177 | 10.205 | 115.372 | 1.00 | 28.73 | AAGL |
| ATOM | 1272 | N | GLY | 164 | 15.448 | 11.613 | 115.598 | 1.00 | 25.57 | AAGL |
| ATOM | 1273 | CA | GLY | 164 | 14.782 | 11.045 | 114.445 | 1.00 | 24.90 | AAGL |
| ATOM | 1274 | C | GLY | 164 | 15.651 | 11.409 | 113.253 | 1.00 | 26.22 | AAGL |
| ATOM | 1275 | O | GLY | 164 | 15.831 | 10.618 | 112.326 | 1.00 | 26.72 | AAGL |
| ATOM | 1276 | N | VAL | 165 | 16.206 | 12.618 | 113.290 | 1.00 | 25.62 | AAGL |
| ATOM | 1277 | CA | VAL | 165 | 17.078 | 13.087 | 112.219 | 1.00 | 26.48 | AAGL |
| ATOM | 1278 | CB | VAL | 165 | 17.379 | 14.598 | 112.356 | 1.00 | 26.61 | AAGL |
| ATOM | 1279 | CG1 | VAL | 165 | 18.398 | 15.026 | 111.293 | 1.00 | 23.67 | AAGL |
| ATOM | 1280 | CG2 | VAL | 165 | 16.090 | 15.397 | 112.216 | 1.00 | 25.11 | AAGL |
| ATOM | 1281 | C | VAL | 165 | 18.406 | 12.328 | 112.251 | 1.00 | 27.69 | AAGL |
| ATOM | 1282 | O | VAL | 165 | 18.850 | 11.788 | 111.233 | 1.00 | 29.75 | AAGL |
| ATOM | 1283 | N | LYS | 166 | 19.037 | 12.295 | 113.420 | 1.00 | 27.66 | AAGL |
| ATOM | 1284 | CA | LYS | 166 | 20.313 | 11.607 | 113.581 | 1.00 | 29.81 | AAGL |
| ATOM | 1285 | CB | LYS | 166 | 20.770 | 11.661 | 115.045 | 1.00 | 29.36 | AAGL |
| ATOM | 1286 | CG | LYS | 166 | 21.062 | 13.060 | 115.590 | 1.00 | 30.72 | AAGL |
| ATOM | 1287 | CD | LYS | 166 | 21.442 | 12.982 | 117.065 | 1.00 | 33.25 | AAGL |
| ATOM | 1288 | CE | LYS | 166 | 21.674 | 14.358 | 117.677 | 1.00 | 33.72 | AAGL |
| ATOM | 1289 | NZ | LYS | 166 | 22.883 | 15.036 | 117.122 | 1.00 | 33.70 | AAGL |
| ATOM | 1290 | C | LYS | 166 | 20.229 | 10.144 | 113.136 | 1.00 | 31.30 | AAGL |
| ATOM | 1291 | O | LYS | 166 | 21.206 | 9.594 | 112.622 | 1.00 | 31.56 | AAGL |
| ATOM | 1292 | N | ASP | 167 | 19.065 | 9.519 | 113.319 | 1.00 | 30.83 | AAGL |
| ATOM | 1293 | CA | ASP | 167 | 18.893 | 8.116 | 112.944 | 1.00 | 32.56 | AAGL |
| ATOM | 1294 | CB | ASP | 167 | 17.863 | 7.442 | 113.854 | 1.00 | 31.71 | AAGL |
| ATOM | 1295 | CG | ASP | 167 | 18.387 | 7.187 | 115.245 | 1.00 | 33.01 | AAGL |
| ATOM | 1296 | OD1 | ASP | 167 | 19.620 | 7.148 | 115.425 | 1.00 | 33.60 | AAGL |
| ATOM | 1297 | OD2 | ASP | 167 | 17.558 | 7.006 | 116.160 | 1.00 | 32.14 | AAGL |
| ATOM | 1298 | C | ASP | 167 | 18.481 | 7.858 | 111.494 | 1.00 | 33.63 | AAGL |
| ATOM | 1299 | O | ASP | 167 | 18.347 | 6.696 | 111.082 | 1.00 | 32.89 | AAGL |
| ATOM | 1300 | N | SER | 168 | 18.280 | 8.925 | 110.724 | 1.00 | 31.74 | AAGL |
| ATOM | 1301 | CA | SER | 168 | 17.846 | 8.786 | 109.341 | 1.00 | 31.90 | AAGL |
| ATOM | 1302 | CB | SER | 168 | 17.279 | 10.111 | 108.823 | 1.00 | 29.91 | AAGL |
| ATOM | 1303 | OG | SER | 168 | 18.301 | 11.074 | 108.654 | 1.00 | 30.10 | AAGL |
| ATOM | 1304 | C | SER | 168 | 18.922 | 8.294 | 108.378 | 1.00 | 32.86 | AAGL |
| ATOM | 1305 | O | SER | 168 | 20.114 | 8.248 | 108.704 | 1.00 | 31.48 | AAGL |
| ATOM | 1306 | N | ASN | 169 | 18.470 | 7.950 | 107.179 | 1.00 | 34.44 | AAGL |
| ATOM | 1307 | CA | ASN | 169 | 19.328 | 7.430 | 106.123 | 1.00 | 37.26 | AAGL |
| ATOM | 1308 | CB | ASN | 169 | 18.493 | 6.545 | 105.195 | 1.00 | 38.60 | AAGL |
| ATOM | 1309 | CG | ASN | 169 | 17.848 | 5.377 | 105.925 | 1.00 | 37.67 | AAGL |
| ATOM | 1310 | OD1 | ASN | 169 | 16.833 | 4.841 | 105.482 | 1.00 | 40.60 | AAGL |
| ATOM | 1311 | ND2 | ASN | 169 | 18.440 | 4.971 | 107.044 | 1.00 | 39.67 | AAGL |
| ATOM | 1312 | C | ASN | 169 | 20.043 | 8.508 | 105.308 | 1.00 | 38.79 | AAGL |
| ATOM | 1313 | O | ASN | 169 | 20.725 | 8.194 | 104.324 | 1.00 | 39.86 | AAGL |
| ATOM | 1314 | N | LEU | 170 | 19.891 | 9.773 | 105.695 | 1.00 | 38.43 | AAGL |
| ATOM | 1315 | CA | LEU | 170 | 20.562 | 10.849 | 104.966 | 1.00 | 39.07 | AAGL |
| ATOM | 1316 | CB | LEU | 170 | 20.133 | 12.222 | 105.502 | 1.00 | 36.50 | AAGL |
| ATOM | 1317 | CG | LEU | 170 | 18.784 | 12.783 | 105.053 | 1.00 | 35.65 | AAGL |
| ATOM | 1318 | CD1 | LEU | 170 | 18.533 | 14.122 | 105.733 | 1.00 | 36.42 | AAGL |
| ATOM | 1319 | CD2 | LEU | 170 | 18.775 | 12.960 | 103.548 | 1.00 | 35.41 | AAGL |
| ATOM | 1320 | C | LEU | 170 | 22.068 | 10.672 | 105.146 | 1.00 | 40.51 | AAGL |
| ATOM | 1321 | O | LEU | 170 | 22.580 | 10.787 | 106.257 | 1.00 | 41.18 | AAGL |
| ATOM | 1322 | N | ALA | 171 | 22.770 | 10.392 | 104.050 | 1.00 | 43.25 | AAGL |
| ATOM | 1323 | CA | ALA | 171 | 24.219 | 10.180 | 104.078 | 1.00 | 44.92 | AAGL |
| ATOM | 1324 | CB | ALA | 171 | 24.796 | 10.430 | 102.700 | 1.00 | 45.32 | AAGL |
| ATOM | 1325 | C | ALA | 171 | 24.913 | 11.063 | 105.117 | 1.00 | 45.99 | AAGL |
| ATOM | 1326 | O | ALA | 171 | 25.671 | 10.568 | 105.962 | 1.00 | 47.05 | AAGL |
| ATOM | 1327 | N | THR | 172 | 24.668 | 12.370 | 105.044 | 1.00 | 46.11 | AAGL |
| ATOM | 1328 | CA | THR | 172 | 25.246 | 13.316 | 105.998 | 1.00 | 45.78 | AAGL |

**Fig. 3 cont.**

| ATOM | 1329 | CB | THR | 172 | 25.856 | 14.549 | 105.320 | 1.00 | 46.89 | AAGL |
|------|------|-----|-----|-----|--------|--------|---------|------|-------|------|
| ATOM | 1330 | OG1 | THR | 172 | 26.551 | 14.167 | 104.132 | 1.00 | 48.14 | AAGL |
| ATOM | 1331 | CG2 | THR | 172 | 26.822 | 15.224 | 106.269 | 1.00 | 46.74 | AAGL |
| ATOM | 1332 | C | THR | 172 | 24.117 | 13.844 | 106.868 | 1.00 | 44.10 | AAGL |
| ATOM | 1333 | O | THR | 172 | 23.086 | 14.272 | 106.351 | 1.00 | 44.98 | AAGL |
| ATOM | 1334 | N | THR | 173 | 24.311 | 13.835 | 108.179 | 1.00 | 42.61 | AAGL |
| ATOM | 1335 | CA | THR | 173 | 23.283 | 14.319 | 109.088 | 1.00 | 39.37 | AAGL |
| ATOM | 1336 | CB | THR | 173 | 23.621 | 13.926 | 110.530 | 1.00 | 39.69 | AAGL |
| ATOM | 1337 | OG1 | THR | 173 | 23.691 | 12.497 | 110.620 | 1.00 | 40.97 | AAGL |
| ATOM | 1338 | CG2 | THR | 173 | 22.555 | 14.436 | 111.494 | 1.00 | 40.31 | AAGL |
| ATOM | 1339 | C | THR | 173 | 23.140 | 15.837 | 108.969 | 1.00 | 36.34 | AAGL |
| ATOM | 1340 | O | THR | 173 | 24.118 | 16.581 | 109.083 | 1.00 | 35.72 | AAGL |
| ATOM | 1341 | N | PRO | 174 | 21.916 | 16.319 | 108.702 | 1.00 | 33.51 | AAGL |
| ATOM | 1342 | CD | PRO | 174 | 20.709 | 15.592 | 108.274 | 1.00 | 33.11 | AAGL |
| ATOM | 1343 | CA | PRO | 174 | 21.728 | 17.766 | 108.580 | 1.00 | 30.76 | AAGL |
| ATOM | 1344 | CB | PRO | 174 | 20.252 | 17.891 | 108.223 | 1.00 | 31.41 | AAGL |
| ATOM | 1345 | CG | PRO | 174 | 19.989 | 16.624 | 107.452 | 1.00 | 33.06 | AAGL |
| ATOM | 1346 | C | PRO | 174 | 22.056 | 18.475 | 109.883 | 1.00 | 27.61 | AAGL |
| ATOM | 1347 | O | PRO | 174 | 22.074 | 17.865 | 110.945 | 1.00 | 26.79 | AAGL |
| ATOM | 1348 | N | LYS | 175 | 22.332 | 19.767 | 109.800 | 1.00 | 28.61 | AAGL |
| ATOM | 1349 | CA | LYS | 175 | 22.614 | 20.541 | 111.001 | 1.00 | 27.46 | AAGL |
| ATOM | 1350 | CB | LYS | 175 | 23.167 | 21.917 | 110.636 | 1.00 | 30.67 | AAGL |
| ATOM | 1351 | CG | LYS | 175 | 24.679 | 22.002 | 110.611 | 1.00 | 35.14 | AAGL |
| ATOM | 1352 | CD | LYS | 175 | 25.286 | 20.926 | 109.751 | 1.00 | 39.94 | AAGL |
| ATOM | 1353 | CE | LYS | 175 | 26.804 | 21.046 | 109.733 | 1.00 | 42.54 | AAGL |
| ATOM | 1354 | NZ | LYS | 175 | 27.396 | 20.867 | 111.091 | 1.00 | 43.56 | AAGL |
| ATOM | 1355 | C | LYS | 175 | 21.267 | 20.693 | 111.695 | 1.00 | 26.21 | AAGL |
| ATOM | 1356 | O | LYS | 175 | 20.297 | 21.096 | 111.068 | 1.00 | 25.54 | AAGL |
| ATOM | 1357 | N | ILE | 176 | 21.209 | 20.350 | 112.975 | 1.00 | 24.86 | AAGL |
| ATOM | 1358 | CA | ILE | 176 | 19.968 | 20.443 | 113.728 | 1.00 | 24.97 | AAGL |
| ATOM | 1359 | CB | ILE | 176 | 19.899 | 19.320 | 114.779 | 1.00 | 25.45 | AAGL |
| ATOM | 1360 | CG2 | ILE | 176 | 18.689 | 19.515 | 115.676 | 1.00 | 25.15 | AAGL |
| ATOM | 1361 | CG1 | ILE | 176 | 19.847 | 17.964 | 114.061 | 1.00 | 25.46 | AAGL |
| ATOM | 1362 | CD1 | ILE | 176 | 20.148 | 16.775 | 114.941 | 1.00 | 26.04 | AAGL |
| ATOM | 1363 | C | ILE | 176 | 19.866 | 21.807 | 114.395 | 1.00 | 23.30 | AAGL |
| ATOM | 1364 | O | ILE | 176 | 20.752 | 22.208 | 115.136 | 1.00 | 24.10 | AAGL |
| ATOM | 1365 | N | MET | 177 | 18.769 | 22.507 | 114.127 | 1.00 | 23.38 | AAGL |
| ATOM | 1366 | CA | MET | 177 | 18.557 | 23.847 | 114.656 | 1.00 | 22.20 | AAGL |
| ATOM | 1367 | CB | MET | 177 | 18.401 | 24.837 | 113.488 | 1.00 | 20.47 | AAGL |
| ATOM | 1368 | CG | MET | 177 | 17.934 | 26.249 | 113.903 | 1.00 | 21.58 | AAGL |
| ATOM | 1369 | SD | MET | 177 | 17.586 | 27.336 | 112.488 | 1.00 | 22.93 | AAGL |
| ATOM | 1370 | CE | MET | 177 | 19.288 | 27.706 | 111.969 | 1.00 | 22.76 | AAGL |
| ATOM | 1371 | C | MET | 177 | 17.352 | 24.013 | 115.576 | 1.00 | 21.82 | AAGL |
| ATOM | 1372 | O | MET | 177 | 16.343 | 23.326 | 115.425 | 1.00 | 21.31 | AAGL |
| ATOM | 1373 | N | ILE | 178 | 17.485 | 24.927 | 116.534 | 1.00 | 20.60 | AAGL |
| ATOM | 1374 | CA | ILE | 178 | 16.395 | 25.294 | 117.433 | 1.00 | 21.53 | AAGL |
| ATOM | 1375 | CB | ILE | 178 | 16.750 | 25.134 | 118.932 | 1.00 | 22.17 | AAGL |
| ATOM | 1376 | CG2 | ILE | 178 | 15.678 | 25.810 | 119.798 | 1.00 | 22.88 | AAGL |
| ATOM | 1377 | CG1 | ILE | 178 | 16.830 | 23.647 | 119.286 | 1.00 | 23.39 | AAGL |
| ATOM | 1378 | CD1 | ILE | 178 | 17.014 | 23.363 | 120.767 | 1.00 | 25.76 | AAGL |
| ATOM | 1379 | C | ILE | 178 | 16.204 | 26.766 | 117.088 | 1.00 | 19.40 | AAGL |
| ATOM | 1380 | O | ILE | 178 | 17.156 | 27.555 | 117.127 | 1.00 | 19.88 | AAGL |
| ATOM | 1381 | N | HIS | 179 | 14.971 | 27.125 | 116.751 | 1.00 | 18.62 | AAGL |
| ATOM | 1382 | CA | HIS | 179 | 14.632 | 28.475 | 116.312 | 1.00 | 18.14 | AAGL |
| ATOM | 1383 | CB | HIS | 179 | 14.054 | 28.356 | 114.899 | 1.00 | 17.60 | AAGL |
| ATOM | 1384 | CG | HIS | 179 | 13.454 | 29.617 | 114.363 | 1.00 | 18.42 | AAGL |
| ATOM | 1385 | CD2 | HIS | 179 | 13.731 | 30.919 | 114.609 | 1.00 | 17.14 | AAGL |
| ATOM | 1386 | ND1 | HIS | 179 | 12.438 | 29.611 | 113.432 | 1.00 | 18.37 | AAGL |
| ATOM | 1387 | CE1 | HIS | 179 | 12.114 | 30.855 | 113.129 | 1.00 | 16.27 | AAGL |
| ATOM | 1388 | NE2 | HIS | 179 | 12.883 | 31.668 | 113.830 | 1.00 | 17.92 | AAGL |
| ATOM | 1389 | C | HIS | 179 | 13.658 | 29.235 | 117.227 | 1.00 | 20.10 | AAGL |
| ATOM | 1390 | O | HIS | 179 | 12.541 | 28.780 | 117.470 | 1.00 | 20.46 | AAGL |
| ATOM | 1391 | N | LEU | 180 | 14.090 | 30.394 | 117.716 | 1.00 | 18.07 | AAGL |
| ATOM | 1392 | CA | LEU | 180 | 13.258 | 31.237 | 118.574 | 1.00 | 19.85 | AAGL |
| ATOM | 1393 | CB | LEU | 180 | 13.930 | 31.480 | 119.928 | 1.00 | 20.54 | AAGL |
| ATOM | 1394 | CG | LEU | 180 | 14.253 | 30.306 | 120.854 | 1.00 | 24.61 | AAGL |
| ATOM | 1395 | CD1 | LEU | 180 | 14.701 | 30.866 | 122.208 | 1.00 | 23.57 | AAGL |

# Fig. 3 cont.

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1396 | CD2 | LEU | 180 | 13.038 | 29.405 | 121.029 | 1.00 | 22.59 | AAGL |
| ATOM | 1397 | C | LEU | 180 | 13.027 | 32.588 | 117.905 | 1.00 | 20.35 | AAGL |
| ATOM | 1398 | O | LEU | 180 | 13.838 | 33.032 | 117.099 | 1.00 | 20.34 | AAGL |
| ATOM | 1399 | N | ASP | 181 | 11.918 | 33.237 | 118.240 | 1.00 | 19.30 | AAGL |
| ATOM | 1400 | CA | ASP | 181 | 11.623 | 34.548 | 117.688 | 1.00 | 19.90 | AAGL |
| ATOM | 1401 | CB | ASP | 181 | 10.112 | 34.796 | 117.680 | 1.00 | 21.15 | AAGL |
| ATOM | 1402 | CG | ASP | 181 | 9.522 | 34.825 | 119.070 | 1.00 | 22.95 | AAGL |
| ATOM | 1403 | OD1 | ASP | 181 | 9.910 | 33.973 | 119.900 | 1.00 | 22.67 | AAGL |
| ATOM | 1404 | OD2 | ASP | 181 | 8.664 | 35.697 | 119.336 | 1.00 | 25.18 | AAGL |
| ATOM | 1405 | C | ASP | 181 | 12.315 | 35.580 | 118.576 | 1.00 | 21.86 | AAGL |
| ATOM | 1406 | O | ASP | 181 | 13.020 | 35.218 | 119.524 | 1.00 | 23.76 | AAGL |
| ATOM | 1407 | N | ASP | 182 | 12.107 | 36.856 | 118.271 | 1.00 | 22.19 | AAGL |
| ATOM | 1408 | CA | ASP | 182 | 12.718 | 37.948 | 119.034 | 1.00 | 22.68 | AAGL |
| ATOM | 1409 | CB | ASP | 182 | 12.013 | 38.129 | 120.381 | 1.00 | 24.73 | AAGL |
| ATOM | 1410 | CG | ASP | 182 | 10.589 | 38.605 | 120.234 | 1.00 | 26.20 | AAGL |
| ATOM | 1411 | OD1 | ASP | 182 | 10.226 | 39.052 | 119.134 | 1.00 | 30.46 | AAGL |
| ATOM | 1412 | OD2 | ASP | 182 | 9.829 | 38.539 | 121.226 | 1.00 | 30.54 | AAGL |
| ATOM | 1413 | C | ASP | 182 | 14.205 | 37.719 | 119.282 | 1.00 | 21.94 | AAGL |
| ATOM | 1414 | O | ASP | 182 | 14.645 | 37.656 | 120.432 | 1.00 | 22.68 | AAGL |
| ATOM | 1415 | N | GLY | 183 | 14.975 | 37.610 | 118.203 | 1.00 | 21.90 | AAGL |
| ATOM | 1416 | CA | GLY | 183 | 16.403 | 37.388 | 118.334 | 1.00 | 20.97 | AAGL |
| ATOM | 1417 | C | GLY | 183 | 17.158 | 38.524 | 119.003 | 1.00 | 21.01 | AAGL |
| ATOM | 1418 | O | GLY | 183 | 18.279 | 38.340 | 119.478 | 1.00 | 24.20 | AAGL |
| ATOM | 1419 | N | TRP | 184 | 16.550 | 39.701 | 119.045 | 1.00 | 23.43 | AAGL |
| ATOM | 1420 | CA | TRP | 184 | 17.191 | 40.859 | 119.655 | 1.00 | 25.63 | AAGL |
| ATOM | 1421 | CB | TRP | 184 | 16.514 | 42.141 | 119.173 | 1.00 | 24.89 | AAGL |
| ATOM | 1422 | CG | TRP | 184 | 15.045 | 42.120 | 119.376 | 1.00 | 27.09 | AAGL |
| ATOM | 1423 | CD2 | TRP | 184 | 14.346 | 42.467 | 120.576 | 1.00 | 28.81 | AAGL |
| ATOM | 1424 | CE2 | TRP | 184 | 12.971 | 42.248 | 120.336 | 1.00 | 28.20 | AAGL |
| ATOM | 1425 | CE3 | TRP | 184 | 14.750 | 42.944 | 121.833 | 1.00 | 30.34 | AAGL |
| ATOM | 1426 | CD1 | TRP | 184 | 14.098 | 41.717 | 118.481 | 1.00 | 27.72 | AAGL |
| ATOM | 1427 | NE1 | TRP | 184 | 12.847 | 41.792 | 119.049 | 1.00 | 27.27 | AAGL |
| ATOM | 1428 | CZ2 | TRP | 184 | 11.994 | 42.487 | 121.308 | 1.00 | 32.25 | AAGL |
| ATOM | 1429 | CZ3 | TRP | 184 | 13.776 | 43.184 | 122.802 | 1.00 | 33.25 | AAGL |
| ATOM | 1430 | CH2 | TRP | 184 | 12.414 | 42.954 | 122.533 | 1.00 | 30.56 | AAGL |
| ATOM | 1431 | C | TRP | 184 | 17.155 | 40.816 | 121.184 | 1.00 | 27.12 | AAGL |
| ATOM | 1432 | O | TRP | 184 | 17.869 | 41.563 | 121.850 | 1.00 | 26.68 | AAGL |
| ATOM | 1433 | N | SER | 185 | 16.332 | 39.935 | 121.742 | 1.00 | 26.77 | AAGL |
| ATOM | 1434 | CA | SER | 185 | 16.207 | 39.846 | 123.190 | 1.00 | 28.56 | AAGL |
| ATOM | 1435 | CB | SER | 185 | 14.739 | 39.648 | 123.558 | 1.00 | 28.06 | AAGL |
| ATOM | 1436 | OG | SER | 185 | 14.594 | 39.465 | 124.949 | 1.00 | 31.97 | AAGL |
| ATOM | 1437 | C | SER | 185 | 17.055 | 38.761 | 123.858 | 1.00 | 27.96 | AAGL |
| ATOM | 1438 | O | SER | 185 | 16.660 | 37.600 | 123.919 | 1.00 | 29.29 | AAGL |
| ATOM | 1439 | N | TRP | 186 | 18.218 | 39.142 | 124.374 | 1.00 | 27.87 | AAGL |
| ATOM | 1440 | CA | TRP | 186 | 19.091 | 38.176 | 125.032 | 1.00 | 27.87 | AAGL |
| ATOM | 1441 | CB | TRP | 186 | 20.380 | 38.853 | 125.511 | 1.00 | 29.10 | AAGL |
| ATOM | 1442 | CG | TRP | 186 | 21.165 | 38.036 | 126.509 | 1.00 | 27.39 | AAGL |
| ATOM | 1443 | CD2 | TRP | 186 | 21.670 | 36.705 | 126.335 | 1.00 | 29.36 | AAGL |
| ATOM | 1444 | CE2 | TRP | 186 | 22.338 | 36.352 | 127.531 | 1.00 | 30.06 | AAGL |
| ATOM | 1445 | CE3 | TRP | 186 | 21.625 | 35.774 | 125.285 | 1.00 | 30.04 | AAGL |
| ATOM | 1446 | CD1 | TRP | 186 | 21.534 | 38.422 | 127.765 | 1.00 | 29.38 | AAGL |
| ATOM | 1447 | NE1 | TRP | 186 | 22.239 | 37.417 | 128.386 | 1.00 | 28.39 | AAGL |
| ATOM | 1448 | CZ2 | TRP | 186 | 22.957 | 35.108 | 127.705 | 1.00 | 30.53 | AAGL |
| ATOM | 1449 | CZ3 | TRP | 186 | 22.240 | 34.540 | 125.459 | 1.00 | 30.87 | AAGL |
| ATOM | 1450 | CH2 | TRP | 186 | 22.898 | 34.218 | 126.662 | 1.00 | 31.05 | AAGL |
| ATOM | 1451 | C | TRP | 186 | 18.418 | 37.486 | 126.217 | 1.00 | 28.13 | AAGL |
| ATOM | 1452 | O | TRP | 186 | 18.620 | 36.291 | 126.445 | 1.00 | 27.04 | AAGL |
| ATOM | 1453 | N | ASP | 187 | 17.628 | 38.232 | 126.979 | 1.00 | 28.09 | AAGL |
| ATOM | 1454 | CA | ASP | 187 | 16.961 | 37.643 | 128.131 | 1.00 | 29.42 | AAGL |
| ATOM | 1455 | CB | ASP | 187 | 16.156 | 38.704 | 128.887 | 1.00 | 32.15 | AAGL |
| ATOM | 1456 | CG | ASP | 187 | 17.028 | 39.817 | 129.450 | 1.00 | 37.52 | AAGL |
| ATOM | 1457 | OD1 | ASP | 187 | 18.255 | 39.612 | 129.611 | 1.00 | 39.29 | AAGL |
| ATOM | 1458 | OD2 | ASP | 187 | 16.476 | 40.896 | 129.748 | 1.00 | 41.44 | AAGL |
| ATOM | 1459 | C | ASP | 187 | 16.035 | 36.488 | 127.724 | 1.00 | 28.91 | AAGL |
| ATOM | 1460 | O | ASP | 187 | 16.033 | 35.431 | 128.357 | 1.00 | 27.77 | AAGL |
| ATOM | 1461 | N | GLN | 188 | 15.250 | 36.691 | 126.668 | 1.00 | 27.43 | AAGL |
| ATOM | 1462 | CA | GLN | 188 | 14.326 | 35.657 | 126.215 | 1.00 | 27.67 | AAGL |

# Fig. 3 cont.

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1463 | CB | GLN | 188 | 13.357 | 36.220 | 125.170 | 1.00 28.11 | AAGL |
| ATOM | 1464 | CG | GLN | 188 | 12.222 | 37.066 | 125.735 | 1.00 31.74 | AAGL |
| ATOM | 1465 | CD | GLN | 188 | 11.247 | 36.258 | 126.588 | 1.00 36.22 | AAGL |
| ATOM | 1466 | OE1 | GLN | 188 | 10.921 | 35.103 | 126.274 | 1.00 36.68 | AAGL |
| ATOM | 1467 | NE2 | GLN | 188 | 10.760 | 36.867 | 127.660 | 1.00 37.18 | AAGL |
| ATOM | 1468 | C | GLN | 188 | 15.061 | 34.456 | 125.641 | 1.00 26.39 | AAGL |
| ATOM | 1469 | O | GLN | 188 | 14.710 | 33.318 | 125.934 | 1.00 26.19 | AAGL |
| ATOM | 1470 | N | GLN | 189 | 16.086 | 34.712 | 124.829 | 1.00 25.52 | AAGL |
| ATOM | 1471 | CA | GLN | 189 | 16.864 | 33.633 | 124.225 | 1.00 24.65 | AAGL |
| ATOM | 1472 | CB | GLN | 189 | 17.997 | 34.191 | 123.351 | 1.00 24.63 | AAGL |
| ATOM | 1473 | CG | GLN | 189 | 17.576 | 34.991 | 122.126 | 1.00 24.46 | AAGL |
| ATOM | 1474 | CD | GLN | 189 | 16.736 | 34.191 | 121.149 | 1.00 21.93 | AAGL |
| ATOM | 1475 | OE1 | GLN | 189 | 17.097 | 33.084 | 120.760 | 1.00 20.15 | AAGL |
| ATOM | 1476 | NE2 | GLN | 189 | 15.613 | 34.759 | 120.739 | 1.00 23.53 | AAGL |
| ATOM | 1477 | C | GLN | 189 | 17.484 | 32.759 | 125.308 | 1.00 25.42 | AAGL |
| ATOM | 1478 | O | GLN | 189 | 17.314 | 31.544 | 125.324 | 1.00 23.58 | AAGL |
| ATOM | 1479 | N | ASN | 190 | 18.199 | 33.405 | 126.219 | 1.00 25.59 | AAGL |
| ATOM | 1480 | CA | ASN | 190 | 18.892 | 32.725 | 127.293 | 1.00 26.28 | AAGL |
| ATOM | 1481 | CB | ASN | 190 | 19.745 | 33.736 | 128.056 | 1.00 28.08 | AAGL |
| ATOM | 1482 | CG | ASN | 190 | 20.593 | 33.091 | 129.135 | 1.00 29.88 | AAGL |
| ATOM | 1483 | OD1 | ASN | 190 | 21.204 | 32.041 | 128.922 | 1.00 29.87 | AAGL |
| ATOM | 1484 | ND2 | ASN | 190 | 20.649 | 33.727 | 130.295 | 1.00 33.02 | AAGL |
| ATOM | 1485 | C | ASN | 190 | 17.978 | 31.970 | 128.250 | 1.00 26.80 | AAGL |
| ATOM | 1486 | O | ASN | 190 | 18.300 | 30.866 | 128.675 | 1.00 27.29 | AAGL |
| ATOM | 1487 | N | TYR | 191 | 16.838 | 32.554 | 128.590 | 1.00 27.59 | AAGL |
| ATOM | 1488 | CA | TYR | 191 | 15.931 | 31.878 | 129.504 | 1.00 27.82 | AAGL |
| ATOM | 1489 | CB | TYR | 191 | 14.735 | 32.767 | 129.832 | 1.00 28.23 | AAGL |
| ATOM | 1490 | CG | TYR | 191 | 13.815 | 32.132 | 130.844 | 1.00 30.08 | AAGL |
| ATOM | 1491 | CD1 | TYR | 191 | 12.775 | 31.294 | 130.446 | 1.00 32.24 | AAGL |
| ATOM | 1492 | CE1 | TYR | 191 | 11.975 | 30.641 | 131.385 | 1.00 33.28 | AAGL |
| ATOM | 1493 | CD2 | TYR | 191 | 14.032 | 32.308 | 132.210 | 1.00 31.47 | AAGL |
| ATOM | 1494 | CE2 | TYR | 191 | 13.240 | 31.662 | 133.157 | 1.00 31.82 | AAGL |
| ATOM | 1495 | CZ | TYR | 191 | 12.219 | 30.830 | 132.739 | 1.00 34.47 | AAGL |
| ATOM | 1496 | OH | TYR | 191 | 11.458 | 30.168 | 133.679 | 1.00 36.38 | AAGL |
| ATOM | 1497 | C | TYR | 191 | 15.443 | 30.551 | 128.929 | 1.00 27.27 | AAGL |
| ATOM | 1498 | O | TYR | 191 | 15.392 | 29.537 | 129.631 | 1.00 25.68 | AAGL |
| ATOM | 1499 | N | PHE | 192 | 15.079 | 30.557 | 127.651 | 1.00 25.48 | AAGL |
| ATOM | 1500 | CA | PHE | 192 | 14.605 | 29.341 | 127.016 | 1.00 26.24 | AAGL |
| ATOM | 1501 | CB | PHE | 192 | 14.260 | 29.593 | 125.541 | 1.00 24.60 | AAGL |
| ATOM | 1502 | CG | PHE | 192 | 13.854 | 28.351 | 124.799 | 1.00 22.89 | AAGL |
| ATOM | 1503 | CD1 | PHE | 192 | 12.541 | 27.893 | 124.848 | 1.00 23.14 | AAGL |
| ATOM | 1504 | CD2 | PHE | 192 | 14.795 | 27.607 | 124.098 | 1.00 22.70 | AAGL |
| ATOM | 1505 | CE1 | PHE | 192 | 12.169 | 26.706 | 124.208 | 1.00 22.64 | AAGL |
| ATOM | 1506 | CE2 | PHE | 192 | 14.439 | 26.417 | 123.455 | 1.00 22.68 | AAGL |
| ATOM | 1507 | CZ | PHE | 192 | 13.125 | 25.965 | 123.510 | 1.00 23.16 | AAGL |
| ATOM | 1508 | C | PHE | 192 | 15.651 | 28.237 | 127.095 | 1.00 26.50 | AAGL |
| ATOM | 1509 | O | PHE | 192 | 15.386 | 27.154 | 127.612 | 1.00 25.06 | AAGL |
| ATOM | 1510 | N | TYR | 193 | 16.847 | 28.513 | 126.577 | 1.00 26.97 | AAGL |
| ATOM | 1511 | CA | TYR | 193 | 17.898 | 27.510 | 126.570 | 1.00 28.47 | AAGL |
| ATOM | 1512 | CB | TYR | 193 | 19.066 | 27.991 | 125.704 | 1.00 25.93 | AAGL |
| ATOM | 1513 | CG | TYR | 193 | 18.675 | 28.113 | 124.243 | 1.00 26.36 | AAGL |
| ATOM | 1514 | CD1 | TYR | 193 | 18.344 | 26.979 | 123.498 | 1.00 24.37 | AAGL |
| ATOM | 1515 | CE1 | TYR | 193 | 17.905 | 27.084 | 122.178 | 1.00 23.29 | AAGL |
| ATOM | 1516 | CD2 | TYR | 193 | 18.561 | 29.357 | 123.632 | 1.00 26.34 | AAGL |
| ATOM | 1517 | CE2 | TYR | 193 | 18.121 | 29.474 | 122.307 | 1.00 24.57 | AAGL |
| ATOM | 1518 | CZ | TYR | 193 | 17.797 | 28.331 | 121.592 | 1.00 23.44 | AAGL |
| ATOM | 1519 | OH | TYR | 193 | 17.370 | 28.431 | 120.290 | 1.00 24.47 | AAGL |
| ATOM | 1520 | C | TYR | 193 | 18.384 | 27.087 | 127.952 | 1.00 28.72 | AAGL |
| ATOM | 1521 | O | TYR | 193 | 18.542 | 25.892 | 128.212 | 1.00 29.46 | AAGL |
| ATOM | 1522 | N | GLU | 194 | 18.610 | 28.046 | 128.844 | 1.00 30.56 | AAGL |
| ATOM | 1523 | CA | GLU | 194 | 19.081 | 27.684 | 130.177 | 1.00 32.74 | AAGL |
| ATOM | 1524 | CB | GLU | 194 | 19.344 | 28.921 | 131.048 | 1.00 36.66 | AAGL |
| ATOM | 1525 | CG | GLU | 194 | 20.119 | 28.543 | 132.325 | 1.00 42.88 | AAGL |
| ATOM | 1526 | CD | GLU | 194 | 20.271 | 29.668 | 133.327 | 1.00 46.55 | AAGL |
| ATOM | 1527 | OE1 | GLU | 194 | 21.086 | 29.502 | 134.275 | 1.00 48.27 | AAGL |
| ATOM | 1528 | OE2 | GLU | 194 | 19.580 | 30.704 | 133.194 | 1.00 47.67 | AAGL |
| ATOM | 1529 | C | GLU | 194 | 18.056 | 26.802 | 130.875 | 1.00 31.54 | AAGL |

**Fig. 3 cont.**

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1530 | O | GLU | 194 | 18.396 | 25.764 | 131.445 | 1.00 | 31.58 | AAGL |
| ATOM | 1531 | N | THR | 195 | 16.795 | 27.212 | 130.823 | 1.00 | 30.56 | AAGL |
| ATOM | 1532 | CA | THR | 195 | 15.731 | 26.453 | 131.468 | 1.00 | 28.40 | AAGL |
| ATOM | 1533 | CB | THR | 195 | 14.408 | 27.226 | 131.402 | 1.00 | 27.94 | AAGL |
| ATOM | 1534 | OG1 | THR | 195 | 14.611 | 28.545 | 131.929 | 1.00 | 25.50 | AAGL |
| ATOM | 1535 | CG2 | THR | 195 | 13.330 | 26.516 | 132.211 | 1.00 | 26.24 | AAGL |
| ATOM | 1536 | C | THR | 195 | 15.535 | 25.054 | 130.868 | 1.00 | 28.06 | AAGL |
| ATOM | 1537 | O | THR | 195 | 15.427 | 24.071 | 131.599 | 1.00 | 26.71 | AAGL |
| ATOM | 1538 | N | VAL | 196 | 15.486 | 24.961 | 129.545 | 1.00 | 27.08 | AAGL |
| ATOM | 1539 | CA | VAL | 196 | 15.301 | 23.666 | 128.902 | 1.00 | 27.16 | AAGL |
| ATOM | 1540 | CB | VAL | 196 | 15.035 | 23.838 | 127.369 | 1.00 | 29.10 | AAGL |
| ATOM | 1541 | CG1 | VAL | 196 | 16.227 | 24.510 | 126.700 | 1.00 | 30.65 | AAGL |
| ATOM | 1542 | CG2 | VAL | 196 | 14.748 | 22.487 | 126.727 | 1.00 | 31.18 | AAGL |
| ATOM | 1543 | C | VAL | 196 | 16.502 | 22.736 | 129.137 | 1.00 | 26.59 | AAGL |
| ATOM | 1544 | O | VAL | 196 | 16.330 | 21.563 | 129.449 | 1.00 | 25.06 | AAGL |
| ATOM | 1545 | N | LEU | 197 | 17.716 | 23.266 | 129.015 | 1.00 | 26.11 | AAGL |
| ATOM | 1546 | CA | LEU | 197 | 18.911 | 22.451 | 129.214 | 1.00 | 28.97 | AAGL |
| ATOM | 1547 | CB | LEU | 197 | 20.161 | 23.207 | 128.735 | 1.00 | 29.84 | AAGL |
| ATOM | 1548 | CG | LEU | 197 | 20.233 | 23.474 | 127.220 | 1.00 | 30.49 | AAGL |
| ATOM | 1549 | CD1 | LEU | 197 | 21.377 | 24.445 | 126.927 | 1.00 | 32.56 | AAGL |
| ATOM | 1550 | CD2 | LEU | 197 | 20.413 | 22.176 | 126.464 | 1.00 | 30.05 | AAGL |
| ATOM | 1551 | C | LEU | 197 | 19.069 | 22.032 | 130.674 | 1.00 | 28.89 | AAGL |
| ATOM | 1552 | O | LEU | 197 | 19.632 | 20.976 | 130.971 | 1.00 | 30.68 | AAGL |
| ATOM | 1553 | N | ALA | 198 | 18.550 | 22.844 | 131.586 | 1.00 | 29.81 | AAGL |
| ATOM | 1554 | CA | ALA | 198 | 18.646 | 22.530 | 133.008 | 1.00 | 30.14 | AAGL |
| ATOM | 1555 | CB | ALA | 198 | 18.110 | 23.688 | 133.831 | 1.00 | 29.46 | AAGL |
| ATOM | 1556 | C | ALA | 198 | 17.913 | 21.237 | 133.387 | 1.00 | 31.06 | AAGL |
| ATOM | 1557 | O | ALA | 198 | 18.223 | 20.624 | 134.411 | 1.00 | 30.62 | AAGL |
| ATOM | 1558 | N | THR | 199 | 16.951 | 20.814 | 132.569 | 1.00 | 30.12 | AAGL |
| ATOM | 1559 | CA | THR | 199 | 16.192 | 19.599 | 132.868 | 1.00 | 29.04 | AAGL |
| ATOM | 1560 | CB | THR | 199 | 14.831 | 19.569 | 132.137 | 1.00 | 30.14 | AAGL |
| ATOM | 1561 | OG1 | THR | 199 | 15.051 | 19.375 | 130.735 | 1.00 | 28.92 | AAGL |
| ATOM | 1562 | CG2 | THR | 199 | 14.058 | 20.876 | 132.351 | 1.00 | 28.52 | AAGL |
| ATOM | 1563 | C | THR | 199 | 16.926 | 18.308 | 132.497 | 1.00 | 30.21 | AAGL |
| ATOM | 1564 | O | THR | 199 | 16.602 | 17.237 | 133.006 | 1.00 | 31.94 | AAGL |
| ATOM | 1565 | N | GLY | 200 | 17.907 | 18.406 | 131.613 | 1.00 | 29.95 | AAGL |
| ATOM | 1566 | CA | GLY | 200 | 18.626 | 17.219 | 131.194 | 1.00 | 30.95 | AAGL |
| ATOM | 1567 | C | GLY | 200 | 17.868 | 16.428 | 130.143 | 1.00 | 31.30 | AAGL |
| ATOM | 1568 | O | GLY | 200 | 18.376 | 15.436 | 129.625 | 1.00 | 31.90 | AAGL |
| ATOM | 1569 | N | GLU | 201 | 16.647 | 16.850 | 129.823 | 1.00 | 31.18 | AAGL |
| ATOM | 1570 | CA | GLU | 201 | 15.856 | 16.145 | 128.813 | 1.00 | 30.31 | AAGL |
| ATOM | 1571 | CB | GLU | 201 | 14.385 | 16.557 | 128.881 | 1.00 | 29.74 | AAGL |
| ATOM | 1572 | CG | GLU | 201 | 13.640 | 16.062 | 130.110 | 1.00 | 32.87 | AAGL |
| ATOM | 1573 | CD | GLU | 201 | 13.710 | 14.555 | 130.285 | 1.00 | 33.76 | AAGL |
| ATOM | 1574 | OE1 | GLU | 201 | 13.838 | 13.833 | 129.274 | 1.00 | 34.18 | AAGL |
| ATOM | 1575 | OE2 | GLU | 201 | 13.617 | 14.086 | 131.443 | 1.00 | 34.63 | AAGL |
| ATOM | 1576 | C | GLU | 201 | 16.399 | 16.440 | 127.423 | 1.00 | 28.94 | AAGL |
| ATOM | 1577 | O | GLU | 201 | 16.271 | 15.625 | 126.511 | 1.00 | 27.79 | AAGL |
| ATOM | 1578 | N | LEU | 202 | 16.988 | 17.623 | 127.272 | 1.00 | 28.10 | AAGL |
| ATOM | 1579 | CA | LEU | 202 | 17.587 | 18.033 | 126.009 | 1.00 | 28.10 | AAGL |
| ATOM | 1580 | CB | LEU | 202 | 17.029 | 19.376 | 125.548 | 1.00 | 28.75 | AAGL |
| ATOM | 1581 | CG | LEU | 202 | 17.766 | 19.987 | 124.350 | 1.00 | 27.26 | AAGL |
| ATOM | 1582 | CD1 | LEU | 202 | 17.461 | 19.196 | 123.090 | 1.00 | 27.62 | AAGL |
| ATOM | 1583 | CD2 | LEU | 202 | 17.337 | 21.430 | 124.178 | 1.00 | 29.02 | AAGL |
| ATOM | 1584 | C | LEU | 202 | 19.088 | 18.170 | 126.240 | 1.00 | 28.79 | AAGL |
| ATOM | 1585 | O | LEU | 202 | 19.518 | 18.888 | 127.141 | 1.00 | 29.33 | AAGL |
| ATOM | 1586 | N | LEU | 203 | 19.875 | 17.473 | 125.433 | 1.00 | 29.74 | AAGL |
| ATOM | 1587 | CA | LEU | 203 | 21.326 | 17.524 | 125.557 | 1.00 | 32.35 | AAGL |
| ATOM | 1588 | CB | LEU | 203 | 21.920 | 16.146 | 125.271 | 1.00 | 33.32 | AAGL |
| ATOM | 1589 | CG | LEU | 203 | 21.643 | 15.084 | 126.328 | 1.00 | 33.68 | AAGL |
| ATOM | 1590 | CD1 | LEU | 203 | 22.436 | 13.828 | 125.998 | 1.00 | 38.12 | AAGL |
| ATOM | 1591 | CD2 | LEU | 203 | 22.053 | 15.615 | 127.694 | 1.00 | 37.93 | AAGL |
| ATOM | 1592 | C | LEU | 203 | 21.934 | 18.541 | 124.603 | 1.00 | 32.26 | AAGL |
| ATOM | 1593 | O | LEU | 203 | 21.475 | 18.694 | 123.474 | 1.00 | 33.19 | AAGL |
| ATOM | 1594 | N | SER | 204 | 22.975 | 19.231 | 125.055 | 1.00 | 33.40 | AAGL |
| ATOM | 1595 | CA | SER | 204 | 23.634 | 20.215 | 124.213 | 1.00 | 34.27 | AAGL |
| ATOM | 1596 | CB | SER | 204 | 24.824 | 20.826 | 124.947 | 1.00 | 34.70 | AAGL |

Fig. 3 cont.

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1597 | OG | SER | 204 | 25.380 | 21.894 | 124.194 | 1.00 | 36.69 | AAGL |
| ATOM | 1598 | C | SER | 204 | 24.103 | 19.529 | 122.934 | 1.00 | 34.03 | AAGL |
| ATOM | 1599 | O | SER | 204 | 24.163 | 20.145 | 121.871 | 1.00 | 35.28 | AAGL |
| ATOM | 1600 | N | THR | 205 | 24.438 | 18.248 | 123.043 | 1.00 | 32.63 | AAGL |
| ATOM | 1601 | CA | THR | 205 | 24.890 | 17.491 | 121.880 | 1.00 | 33.11 | AAGL |
| ATOM | 1602 | CB | THR | 205 | 25.650 | 16.204 | 122.302 | 1.00 | 33.97 | AAGL |
| ATOM | 1603 | OG1 | THR | 205 | 24.875 | 15.458 | 123.256 | 1.00 | 35.21 | AAGL |
| ATOM | 1604 | CG2 | THR | 205 | 26.989 | 16.572 | 122.919 | 1.00 | 34.51 | AAGL |
| ATOM | 1605 | C | THR | 205 | 23.737 | 17.111 | 120.951 | 1.00 | 32.07 | AAGL |
| ATOM | 1606 | O | THR | 205 | 23.960 | 16.584 | 119.865 | 1.00 | 32.54 | AAGL |
| ATOM | 1607 | N | ASP | 206 | 22.504 | 17.389 | 121.367 | 1.00 | 30.83 | AAGL |
| ATOM | 1608 | CA | ASP | 206 | 21.352 | 17.054 | 120.536 | 1.00 | 29.51 | AAGL |
| ATOM | 1609 | CB | ASP | 206 | 20.060 | 17.033 | 121.351 | 1.00 | 28.56 | AAGL |
| ATOM | 1610 | CG | ASP | 206 | 19.996 | 15.871 | 122.315 | 1.00 | 31.99 | AAGL |
| ATOM | 1611 | OD1 | ASP | 206 | 20.539 | 14.791 | 121.990 | 1.00 | 30.07 | AAGL |
| ATOM | 1612 | OD2 | ASP | 206 | 19.385 | 16.037 | 123.390 | 1.00 | 30.30 | AAGL |
| ATOM | 1613 | C | ASP | 206 | 21.151 | 17.986 | 119.352 | 1.00 | 28.75 | AAGL |
| ATOM | 1614 | O | ASP | 206 | 20.514 | 17.597 | 118.376 | 1.00 | 29.56 | AAGL |
| ATOM | 1615 | N | PHE | 207 | 21.653 | 19.217 | 119.437 | 1.00 | 27.57 | AAGL |
| ATOM | 1616 | CA | PHE | 207 | 21.496 | 20.147 | 118.321 | 1.00 | 27.18 | AAGL |
| ATOM | 1617 | CB | PHE | 207 | 20.315 | 21.106 | 118.567 | 1.00 | 24.79 | AAGL |
| ATOM | 1618 | CG | PHE | 207 | 20.541 | 22.115 | 119.651 | 1.00 | 24.63 | AAGL |
| ATOM | 1619 | CD1 | PHE | 207 | 20.643 | 21.728 | 120.981 | 1.00 | 26.07 | AAGL |
| ATOM | 1620 | CD2 | PHE | 207 | 20.613 | 23.473 | 119.341 | 1.00 | 26.18 | AAGL |
| ATOM | 1621 | CE1 | PHE | 207 | 20.811 | 22.677 | 121.986 | 1.00 | 23.87 | AAGL |
| ATOM | 1622 | CE2 | PHE | 207 | 20.782 | 24.433 | 120.340 | 1.00 | 24.35 | AAGL |
| ATOM | 1623 | CZ | PHE | 207 | 20.880 | 24.032 | 121.661 | 1.00 | 26.22 | AAGL |
| ATOM | 1624 | C | PHE | 207 | 22.767 | 20.917 | 117.974 | 1.00 | 27.60 | AAGL |
| ATOM | 1625 | O | PHE | 207 | 23.700 | 20.987 | 118.772 | 1.00 | 28.27 | AAGL |
| ATOM | 1626 | N | ASP | 208 | 22.784 | 21.503 | 116.780 | 1.00 | 28.39 | AAGL |
| ATOM | 1627 | CA | ASP | 208 | 23.958 | 22.209 | 116.278 | 1.00 | 28.84 | AAGL |
| ATOM | 1628 | CB | ASP | 208 | 24.329 | 21.618 | 114.918 | 1.00 | 28.97 | AAGL |
| ATOM | 1629 | CG | ASP | 208 | 24.337 | 20.102 | 114.930 | 1.00 | 29.39 | AAGL |
| ATOM | 1630 | OD1 | ASP | 208 | 25.139 | 19.521 | 115.686 | 1.00 | 30.72 | AAGL |
| ATOM | 1631 | OD2 | ASP | 208 | 23.537 | 19.494 | 114.187 | 1.00 | 30.15 | AAGL |
| ATOM | 1632 | C | ASP | 208 | 23.910 | 23.737 | 116.143 | 1.00 | 28.85 | AAGL |
| ATOM | 1633 | O | ASP | 208 | 24.866 | 24.418 | 116.520 | 1.00 | 28.49 | AAGL |
| ATOM | 1634 | N | TYR | 209 | 22.817 | 24.263 | 115.595 | 1.00 | 26.19 | AAGL |
| ATOM | 1635 | CA | TYR | 209 | 22.674 | 25.704 | 115.368 | 1.00 | 25.08 | AAGL |
| ATOM | 1636 | CB | TYR | 209 | 22.353 | 26.001 | 113.896 | 1.00 | 26.01 | AAGL |
| ATOM | 1637 | CG | TYR | 209 | 23.397 | 25.677 | 112.854 | 1.00 | 23.51 | AAGL |
| ATOM | 1638 | CD1 | TYR | 209 | 24.728 | 25.427 | 113.191 | 1.00 | 27.73 | AAGL |
| ATOM | 1639 | CE1 | TYR | 209 | 25.693 | 25.222 | 112.194 | 1.00 | 27.06 | AAGL |
| ATOM | 1640 | CD2 | TYR | 209 | 23.056 | 25.705 | 111.506 | 1.00 | 26.41 | AAGL |
| ATOM | 1641 | CE2 | TYR | 209 | 24.007 | 25.503 | 110.505 | 1.00 | 29.44 | AAGL |
| ATOM | 1642 | CZ | TYR | 209 | 25.318 | 25.267 | 110.856 | 1.00 | 25.86 | AAGL |
| ATOM | 1643 | OH | TYR | 209 | 26.244 | 25.103 | 109.853 | 1.00 | 26.38 | AAGL |
| ATOM | 1644 | C | TYR | 209 | 21.578 | 26.398 | 116.163 | 1.00 | 23.78 | AAGL |
| ATOM | 1645 | O | TYR | 209 | 20.611 | 25.774 | 116.589 | 1.00 | 23.59 | AAGL |
| ATOM | 1646 | N | PHE | 210 | 21.745 | 27.711 | 116.315 | 1.00 | 25.60 | AAGL |
| ATOM | 1647 | CA | PHE | 210 | 20.775 | 28.584 | 116.969 | 1.00 | 24.58 | AAGL |
| ATOM | 1648 | CB | PHE | 210 | 21.441 | 29.576 | 117.918 | 1.00 | 25.18 | AAGL |
| ATOM | 1649 | CG | PHE | 210 | 21.826 | 29.004 | 119.234 | 1.00 | 26.35 | AAGL |
| ATOM | 1650 | CD1 | PHE | 210 | 20.895 | 28.309 | 120.004 | 1.00 | 26.01 | AAGL |
| ATOM | 1651 | CD2 | PHE | 210 | 23.104 | 29.214 | 119.741 | 1.00 | 26.73 | AAGL |
| ATOM | 1652 | CE1 | PHE | 210 | 21.234 | 27.836 | 121.269 | 1.00 | 28.08 | AAGL |
| ATOM | 1653 | CE2 | PHE | 210 | 23.453 | 28.746 | 121.000 | 1.00 | 29.00 | AAGL |
| ATOM | 1654 | CZ | PHE | 210 | 22.519 | 28.057 | 121.768 | 1.00 | 28.84 | AAGL |
| ATOM | 1655 | C | PHE | 210 | 20.167 | 29.402 | 115.842 | 1.00 | 25.37 | AAGL |
| ATOM | 1656 | O | PHE | 210 | 20.894 | 29.932 | 115.005 | 1.00 | 26.01 | AAGL |
| ATOM | 1657 | N | GLY | 211 | 18.845 | 29.514 | 115.817 | 1.00 | 22.48 | AAGL |
| ATOM | 1658 | CA | GLY | 211 | 18.214 | 30.313 | 114.784 | 1.00 | 21.15 | AAGL |
| ATOM | 1659 | C | GLY | 211 | 17.305 | 31.333 | 115.441 | 1.00 | 20.32 | AAGL |
| ATOM | 1660 | O | GLY | 211 | 16.631 | 31.007 | 116.412 | 1.00 | 22.35 | AAGL |
| ATOM | 1661 | N | VAL | 212 | 17.285 | 32.560 | 114.931 | 1.00 | 20.60 | AAGL |
| ATOM | 1662 | CA | VAL | 212 | 16.428 | 33.595 | 115.501 | 1.00 | 19.19 | AAGL |
| ATOM | 1663 | CB | VAL | 212 | 17.206 | 34.592 | 116.400 | 1.00 | 20.57 | AAGL |

# Fig. 3 cont.

| ATOM | 1664 | CG1 | VAL | 212 | 17.920 | 33.859 | 117.512 | 1.00 | 21.04 | AAGL |
|------|------|-----|-----|-----|--------|--------|---------|------|-------|------|
| ATOM | 1665 | CG2 | VAL | 212 | 18.169 | 35.419 | 115.554 | 1.00 | 22.31 | AAGL |
| ATOM | 1666 | C   | VAL | 212 | 15.781 | 34.426 | 114.410 | 1.00 | 19.78 | AAGL |
| ATOM | 1667 | O   | VAL | 212 | 16.358 | 34.616 | 113.339 | 1.00 | 19.10 | AAGL |
| ATOM | 1668 | N   | SER | 213 | 14.581 | 34.914 | 114.692 | 1.00 | 18.35 | AAGL |
| ATOM | 1669 | CA  | SER | 213 | 13.869 | 35.775 | 113.758 | 1.00 | 19.01 | AAGL |
| ATOM | 1670 | CB  | SER | 213 | 12.353 | 35.630 | 113.933 | 1.00 | 18.11 | AAGL |
| ATOM | 1671 | OG  | SER | 213 | 11.934 | 34.305 | 113.696 | 1.00 | 17.61 | AAGL |
| ATOM | 1672 | C   | SER | 213 | 14.277 | 37.187 | 114.148 | 1.00 | 18.11 | AAGL |
| ATOM | 1673 | O   | SER | ·213 | 14.506 | 37.461 | 115.323 | 1.00 | 21.77 | AAGL |
| ATOM | 1674 | N   | TYR | 214 | 14.384 | 38.081 | 113.174 | 1.00 | 17.30 | AAGL |
| ATOM | 1675 | CA  | TYR | 214 | 14.744 | 39.458 | 113.478 | 1.00 | 17.43 | AAGL |
| ATOM | 1676 | CB  | TYR | 214 | 16.252 | 39.688 | 113.352 | 1.00 | 19.55 | AAGL |
| ATOM | 1677 | CG  | TYR | 214 | 16.647 | 41.122 | 113.624 | 1.00 | 18.83 | AAGL |
| ATOM | 1678 | CD1 | TYR | 214 | 16.558 | 41.661 | 114.911 | 1.00 | 22.19 | AAGL |
| ATOM | 1679 | CE1 | TYR | 214 | 16.872 | 43.004 | 115.158 | 1.00 | 22.03 | AAGL |
| ATOM | 1680 | CD2 | TYR | 214 | 17.063 | 41.959 | 112.590 | 1.00 | 23.69 | AAGL |
| ATOM | 1681 | CE2 | TYR | 214 | 17.381 | 43.307 | 112.828 | 1.00 | 22.60 | AAGL |
| ATOM | 1682 | CZ  | TYR | 214 | 17.279 | 43.816 | 114.113 | 1.00 | 22.17 | AAGL |
| ATOM | 1683 | OH  | TYR | 214 | 17.561 | 45.141 | 114.346 | 1.00 | 24.19 | AAGL |
| ATOM | 1684 | C   | TYR | 214 | 14.013 | 40.386 | 112.534 | 1.00 | 18.48 | AAGL |
| ATOM | 1685 | O   | TYR | 214 | 14.361 | 40.488 | 111.358 | 1.00 | 18.33 | AAGL |
| ATOM | 1686 | N   | TYR | 215 | 12.990 | 41.048 | 113.067 | 1.00 | 18.28 | AAGL |
| ATOM | 1687 | CA  | TYR | 215 | 12.171 | 41.979 | 112.311 | 1.00 | 16.96 | AAGL |
| ATOM | 1688 | CB  | TYR | 215 | 10.717 | 41.506 | 112.321 | 1.00 | 16.58 | AAGL |
| ATOM | 1689 | CG  | TYR | 215 | 10.497 | 40.277 | 111.465 | 1.00 | 16.72 | AAGL |
| ATOM | 1690 | CD1 | TYR | 215 | 10.456 | 40.377 | 110.075 | 1.00 | 19.62 | AAGL |
| ATOM | 1691 | CE1 | TYR | 215 | 10.264 | 39.252 | 109.274 | 1.00 | 18.54 | AAGL |
| ATOM | 1692 | CD2 | TYR | 215 | 10.346 | 39.013 | 112.038 | 1.00 | 16.88 | AAGL |
| ATOM | 1693 | CE2 | TYR | 215 | 10.156 | 37.875 | 111.245 | 1.00 | 17.19 | AAGL |
| ATOM | 1694 | CZ  | TYR | 215 | 10.111 | 38.007 | 109.862 | 1.00 | 16.90 | AAGL |
| ATOM | 1695 | OH  | TYR | 215 | 9.868  | 36.910 | 109.064 | 1.00 | 17.46 | AAGL |
| ATOM | 1696 | C   | TYR | 215 | 12.297 | 43.374 | 112.920 | 1.00 | 19.56 | AAGL |
| ATOM | 1697 | O   | TYR | 215 | 12.487 | 43.523 | 114.124 | 1.00 | 19.95 | AAGL |
| ATOM | 1698 | N   | PRO | 216 | 12.184 | 44.418 | 112.087 | 1.00 | 20.63 | AAGL |
| ATOM | 1699 | CD  | PRO | 216 | 12.160 | 44.396 | 110.613 | 1.00 | 20.25 | AAGL |
| ATOM | 1700 | CA  | PRO | 216 | 12.308 | 45.788 | 112.589 | 1.00 | 20.50 | AAGL |
| ATOM | 1701 | CB  | PRO | 216 | 13.033 | 46.476 | 111.450 | 1.00 | 22.26 | AAGL |
| ATOM | 1702 | CG  | PRO | 216 | 12.318 | 45.881 | 110.243 | 1.00 | 20.29 | AAGL |
| ATOM | 1703 | C   | PRO | 216 | 11.005 | 46.503 | 112.922 | ·1.00 | 21.80 | AAGL |
| ATOM | 1704 | O   | PRO | 216 | 11.021 | 47.552 | 113.569 | 1.00 | 23.06 | AAGL |
| ATOM | 1705 | N   | PHE | 217 | 9.885  | 45.934 | 112.495 | 1.00 | 20.15 | AAGL |
| ATOM | 1706 | CA  | PHE | 217 | 8.599  | 46.580 | 112.682 | 1.00 | 19.12 | AAGL |
| ATOM | 1707 | CB  | PHE | 217 | 7.940  | 46.729 | 111.308 | 1.00 | 21.27 | AAGL |
| ATOM | 1708 | CG  | PHE | 217 | 8.166  | 45.548 | 110.390 | 1.00 | 22.97 | AAGL |
| ATOM | 1709 | CD1 | PHE | 217 | 7.783  | 44.263 | 110.773 | 1.00 | 22.42 | AAGL |
| ATOM | 1710 | CD2 | PHE | 217 | 8.733  | 45.730 | 109.129 | 1.00 | 24.02 | AAGL |
| ATOM | 1711 | CE1 | PHE | 217 | 7.953  | 43.177 | 109.912 | 1.00 | 22.58 | AAGL |
| ATOM | 1712 | CE2 | PHE | 217 | 8.910  | 44.651 | 108.260 | 1.00 | 22.45 | AAGL |
| ATOM | 1713 | CZ  | PHE | 217 | 8.518  | 43.372 | 108.652 | 1.00 | 22.51 | AAGL |
| ATOM | 1714 | C   | PHE | 217 | 7.586  | 46.016 | 113.671 | 1.00 | 20.44 | AAGL |
| ATOM | 1715 | O   | PHE | 217 | 6.391  | 46.271 | 113.523 | 1.00 | 21.67 | AAGL |
| ATOM | 1716 | N   | TYR | 218 | 8.040  | 45.270 | 114.676 | 1.00 | 22.47 | AAGL |
| ATOM | 1717 | CA  | TYR | 218 | 7.130  | 44.715 | 115.688 | 1.00 | 23.80 | AAGL |
| ATOM | 1718 | CB  | TYR | 218 | 7.155  | 43.177 | 115.681 | 1.00 | 24.44 | AAGL |
| ATOM | 1719 | CG  | TYR | 218 | 6.583  | 42.525 | 114.439 | 1.00 | 21.12 | AAGL |
| ATOM | 1720 | CD1 | TYR | 218 | 5.331  | 42.891 | 113.952 | 1.00 | 22.80 | AAGL |
| ATOM | 1721 | CE1 | TYR | 218 | 4.789  | 42.281 | 112.815 | 1.00 | 25.22 | AAGL |
| ATOM | 1722 | CD2 | TYR | 218 | 7.286  | 41.528 | 113.763 | 1.00 | 23.62 | AAGL |
| ATOM | 1723 | CE2 | TYR | 218 | 6.753  | 40.910 | 112.625 | 1.00 | 23.28 | AAGL |
| ATOM | 1724 | CZ  | TYR | 218 | 5.504  | 41.294 | 112.159 | 1.00 | 24.22 | AAGL |
| ATOM | 1725 | OH  | TYR | 218 | 4.970  | 40.698 | 111.038 | 1.00 | 24.13 | AAGL |
| ATOM | 1726 | C   | TYR | 218 | 7.493  | 45.201 | 117.089 | 1.00 | 26.28 | AAGL |
| ATOM | 1727 | O   | TYR | 218 | 6.956  | 44.707 | 118.087 | 1.00 | 28.68 | AAGL |
| ATOM | 1728 | N   | SER | 219 | 8.407  | 46.163 | 117.165 | 1.00 | 27.77 | AAGL |
| ATOM | 1729 | CA  | SER | 219 | 8.854  | 46.712 | 118.447 | 1.00 | 28.32 | AAGL |
| ATOM | 1730 | CB  | SER | 219 | 9.124  | 45.592 | 119.457 | 1.00 | 29.25 | AAGL |

## Fig. 3 cont.

| ATOM | 1731 | OG  | SER | 219 | 9.908  | 46.078 | 120.538 | 1.00 | 31.84 | AAGL |
|------|------|-----|-----|-----|--------|--------|---------|------|-------|------|
| ATOM | 1732 | C   | SER | 219 | 10.119 | 47.549 | 118.303 | 1.00 | 28.53 | AAGL |
| ATOM | 1733 | O   | SER | 219 | 11.107 | 47.110 | 117.716 | 1.00 | 26.20 | AAGL |
| ATOM | 1734 | N   | ALA | 220 | 10.090 | 48.750 | 118.870 | 1.00 | 29.00 | AAGL |
| ATOM | 1735 | CA  | ALA | 220 | 11.235 | 49.647 | 118.816 | 1.00 | 28.92 | AAGL |
| ATOM | 1736 | CB  | ALA | 220 | 10.851 | 51.003 | 119.371 | 1.00 | 28.98 | AAGL |
| ATOM | 1737 | C   | ALA | 220 | 12.440 | 49.104 | 119.572 | 1.00 | 29.06 | AAGL |
| ATOM | 1738 | O   | ALA | 220 | 13.520 | 49.683 | 119.507 | 1.00 | 30.49 | AAGL |
| ATOM | 1739 | N   | SER | 221 | 12.260 | 48.003 | 120.293 | 1.00 | 29.58 | AAGL |
| ATOM | 1740 | CA  | SER | 221 | 13.358 | 47.404 | 121.046 | 1.00 | 29.31 | AAGL |
| ATOM | 1741 | CB  | SER | 221 | 12.815 | 46.522 | 122.169 | 1.00 | 29.65 | AAGL |
| ATOM | 1742 | OG  | SER | 221 | 12.148 | 47.295 | 123.152 | 1.00 | 33.54 | AAGL |
| ATOM | 1743 | C   | SER | 221 | 14.278 | 46.565 | 120.160 | 1.00 | 27.63 | AAGL |
| ATOM | 1744 | O   | SER | 221 | 15.375 | 46.201 | 120.570 | 1.00 | 27.79 | AAGL |
| ATOM | 1745 | N   | ALA | 222 | 13.828 | 46.264 | 118.948 | 1.00 | 26.73 | AAGL |
| ATOM | 1746 | CA  | ALA | 222 | 14.598 | 45.445 | 118.017 | 1.00 | 25.72 | AAGL |
| ATOM | 1747 | CB  | ALA | 222 | 13.662 | 44.864 | 116.953 | 1.00 | 24.78 | AAGL |
| ATOM | 1748 | C   | ALA | 222 | 15.764 | 46.187 | 117.347 | 1.00 | 26.39 | AAGL |
| ATOM | 1749 | O   | ALA | 222 | 15.889 | 46.189 | 116.117 | 1.00 | 24.72 | AAGL |
| ATOM | 1750 | N   | THR | 223 | 16.619 | 46.809 | 118.157 | 1.00 | 25.12 | AAGL |
| ATOM | 1751 | CA  | THR | 223 | 17.771 | 47.536 | 117.632 | 1.00 | 26.47 | AAGL |
| ATOM | 1752 | CB  | THR | 223 | 18.360 | 48.498 | 118.678 | 1.00 | 26.69 | AAGL |
| ATOM | 1753 | OG1 | THR | 223 | 18.793 | 47.749 | 119.822 | 1.00 | 28.21 | AAGL |
| ATOM | 1754 | CG2 | THR | 223 | 17.321 | 49.520 | 119.104 | 1.00 | 25.83 | AAGL |
| ATOM | 1755 | C   | THR | 223 | 18.877 | 46.573 | 117.223 | 1.00 | 25.83 | AAGL |
| ATOM | 1756 | O   | THR | 223 | 18.982 | 45.465 | 117.751 | 1.00 | 28.38 | AAGL |
| ATOM | 1757 | N   | LEU | 224 | 19.703 | 47.000 | 116.278 | 1.00 | 26.34 | AAGL |
| ATOM | 1758 | CA  | LEU | 224 | 20.807 | 46.177 | 115.817 | 1.00 | 27.64 | AAGL |
| ATOM | 1759 | CB  | LEU | 224 | 21.516 | 46.857 | 114.647 | 1.00 | 30.65 | AAGL |
| ATOM | 1760 | CG  | LEU | 224 | 20.769 | 46.842 | 113.311 | 1.00 | 31.90 | AAGL |
| ATOM | 1761 | CD1 | LEU | 224 | 21.565 | 47.603 | 112.257 | 1.00 | 32.52 | AAGL |
| ATOM | 1762 | CD2 | LEU | 224 | 20.558 | 45.406 | 112.873 | 1.00 | 32.19 | AAGL |
| ATOM | 1763 | C   | LEU | 224 | 21.781 | 45.958 | 116.967 | 1.00 | 28.76 | AAGL |
| ATOM | 1764 | O   | LEU | 224 | 22.495 | 44.956 | 117.011 | 1.00 | 30.90 | AAGL |
| ATOM | 1765 | N   | ALA | 225 | 21.796 | 46.902 | 117.903 | 1.00 | 29.40 | AAGL |
| ATOM | 1766 | CA  | ALA | 225 | 22.663 | 46.833 | 119.070 | 1.00 | 29.81 | AAGL |
| ATOM | 1767 | CB  | ALA | 225 | 22.632 | 48.163 | 119.812 | 1.00 | 31.20 | AAGL |
| ATOM | 1768 | C   | ALA | 225 | 22.252 | 45.701 | 120.013 | 1.00 | 30.35 | AAGL |
| ATOM | 1769 | O   | ALA | 225 | 23.105 | 45.003 | 120.560 | 1.00 | 29.58 | AAGL |
| ATOM | 1770 | N   | SER | 226 | 20.948 | 45.526 | 120.215 | 1.00 | 30.66 | AAGL |
| ATOM | 1771 | CA  | SER | 226 | 20.472 | 44.454 | 121.090 | 1.00 | 30.00 | AAGL |
| ATOM | 1772 | CB  | SER | 226 | 18.995 | 44.642 | 121.423 | 1.00 | 30.27 | AAGL |
| ATOM | 1773 | OG  | SER | 226 | 18.851 | 45.426 | 122.592 | 1.00 | 34.03 | AAGL |
| ATOM | 1774 | C   | SER | 226 | 20.685 | 43.096 | 120.437 | 1.00 | 27.61 | AAGL |
| ATOM | 1775 | O   | SER | 226 | 21.003 | 42.114 | 121.113 | 1.00 | 27.38 | AAGL |
| ATOM | 1776 | N   | LEU | 227 | 20.510 | 43.053 | 119.119 | 1.00 | 26.75 | AAGL |
| ATOM | 1777 | CA  | LEU | 227 | 20.691 | 41.828 | 118.359 | 1.00 | 27.51 | AAGL |
| ATOM | 1778 | CB  | LEU | 227 | 20.337 | 42.060 | 116.884 | 1.00 | 25.07 | AAGL |
| ATOM | 1779 | CG  | LEU | 227 | 20.555 | 40.857 | 115.967 | 1.00 | 24.78 | AAGL |
| ATOM | 1780 | CD1 | LEU | 227 | 19.578 | 39.755 | 116.340 | 1.00 | 24.45 | AAGL |
| ATOM | 1781 | CD2 | LEU | 227 | 20.374 | 41.268 | 114.514 | 1.00 | 23.51 | AAGL |
| ATOM | 1782 | C   | LEU | 227 | 22.148 | 41.407 | 118.465 | 1.00 | 28.41 | AAGL |
| ATOM | 1783 | O   | LEU | 227 | 22.456 | 40.253 | 118.726 | 1.00 | 28.87 | AAGL |
| ATOM | 1784 | N   | LYS | 228 | 23.037 | 42.372 | 118.256 | 1.00 | 30.45 | AAGL |
| ATOM | 1785 | CA  | LYS | 228 | 24.474 | 42.132 | 118.316 | 1.00 | 31.96 | AAGL |
| ATOM | 1786 | CB  | LYS | 228 | 25.201 | 43.469 | 118.150 | 1.00 | 36.24 | AAGL |
| ATOM | 1787 | CG  | LYS | 228 | 26.700 | 43.390 | 117.906 | 1.00 | 41.65 | AAGL |
| ATOM | 1788 | CD  | LYS | 228 | 27.242 | 44.757 | 117.477 | 1.00 | 43.74 | AAGL |
| ATOM | 1789 | CE  | LYS | 228 | 26.876 | 45.827 | 118.489 | 1.00 | 46.64 | AAGL |
| ATOM | 1790 | NZ  | LYS | 228 | 27.322 | 47.191 | 118.075 | 1.00 | 47.80 | AAGL |
| ATOM | 1791 | C   | LYS | 228 | 24.820 | 41.485 | 119.653 | 1.00 | 30.16 | AAGL |
| ATOM | 1792 | O   | LYS | 228 | 25.538 | 40.484 | 119.710 | 1.00 | 31.36 | AAGL |
| ATOM | 1793 | N   | THR | 229 | 24.299 | 42.056 | 120.732 | 1.00 | 29.71 | AAGL |
| ATOM | 1794 | CA  | THR | 229 | 24.553 | 41.532 | 122.063 | 1.00 | 30.66 | AAGL |
| ATOM | 1795 | CB  | THR | 229 | 23.981 | 42.452 | 123.142 | 1.00 | 31.91 | AAGL |
| ATOM | 1796 | OG1 | THR | 229 | 24.783 | 43.637 | 123.232 | 1.00 | 35.38 | AAGL |
| ATOM | 1797 | CG2 | THR | 229 | 23.978 | 41.748 | 124.483 | 1.00 | 34.76 | AAGL |

**Fig. 3 cont.**

| ATOM | 1798 | C | THR | 229 | 23.973 | 40.145 | 122.282 | 1.00 | 30.52 | AAGL |
|------|------|------|-----|-----|--------|--------|---------|------|-------|------|
| ATOM | 1799 | O | THR | 229 | 24.615 | 39.290 | 122.883 | 1.00 | 30.20 | AAGL |
| ATOM | 1800 | N | SER | 230 | 22.753 | 39.932 | 121.795 | 1.00 | 29.88 | AAGL |
| ATOM | 1801 | CA | SER | 230 | 22.077 | 38.646 | 121.948 | 1.00 | 27.75 | AAGL |
| ATOM | 1802 | CB | SER | 230 | 20.626 | 38.766 | 121.470 | 1.00 | 27.43 | AAGL |
| ATOM | 1803 | OG | SER | 230 | 19.947 | 37.532 | 121.612 | 1.00 | 28.20 | AAGL |
| ATOM | 1804 | C | SER | 230 | 22.790 | 37.534 | 121.178 | 1.00 | 27.11 | AAGL |
| ATOM | 1805 | O | SER | 230 | 22.994 | 36.436 | 121.698 | 1.00 | 27.65 | AAGL |
| ATOM | 1806 | N | LEU | 231 | 23.157 | 37.814 | 119.935 | 1.00 | 27.30 | AAGL |
| ATOM | 1807 | CA | LEU | 231 | 23.859 | 36.829 | 119.122 | 1.00 | 28.25 | AAGL |
| ATOM | 1808 | CB | LEU | 231 | 24.037 | 37.341 | 117.687 | 1.00 | 28.04 | AAGL |
| ATOM | 1809 | CG | LEU | 231 | 22.767 | 37.430 | 116.832 | 1.00 | 28.82 | AAGL |
| ATOM | 1810 | CD1 | LEU | 231 | 23.091 | 38.027 | 115.468 | 1.00 | 29.62 | AAGL |
| ATOM | 1811 | CD2 | LEU | 231 | 22.171 | 36.034 | 116.670 | 1.00 | 25.68 | AAGL |
| ATOM | 1812 | C | LEU | 231 | 25.228 | 36.541 | 119.733 | 1.00 | 29.07 | AAGL |
| ATOM | 1813 | O | LEU | 231 | 25.685 | 35.399 | 119.743 | 1.00 | 27.21 | AAGL |
| ATOM | 1814 | N | ALA | 232 | 25.874 | 37.585 | 120.244 | 1.00 | 30.00 | AAGL |
| ATOM | 1815 | CA | ALA | 232 | 27.198 | 37.449 | 120.849 | 1.00 | 31.64 | AAGL |
| ATOM | 1816 | CB | ALA | 232 | 27.733 | 38.828 | 121.257 | 1.00 | 30.69 | AAGL |
| ATOM | 1817 | C | ALA | 232 | 27.142 | 36.535 | 122.063 | 1.00 | 31.96 | AAGL |
| ATOM | 1818 | O | ALA | 232 | 27.980 | 35.645 | 122.229 | 1.00 | 32.99 | AAGL |
| ATOM | 1819 | N | ASN | 233 | 26.146 | 36.757 | 122.913 | 1.00 | 31.75 | AAGL |
| ATOM | 1820 | CA | ASN | 233 | 25.989 | 35.960 | 124.118 | 1.00 | 33.65 | AAGL |
| ATOM | 1821 | CB | ASN | 233 | 25.010 | 36.646 | 125.071 | 1.00 | 33.95 | AAGL |
| ATOM | 1822 | CG | ASN | 233 | 25.507 | 38.010 | 125.528 | 1.00 | 37.26 | AAGL |
| ATOM | 1823 | OD1 | ASN | 233 | 26.712 | 38.267 | 125.547 | 1.00 | 37.11 | AAGL |
| ATOM | 1824 | ND2 | ASN | 233 | 24.582 | 38.884 | 125.912 | 1.00 | 37.35 | AAGL |
| ATOM | 1825 | C | ASN | 233 | 25.558 | 34.513 | 123.866 | 1.00 | 33.38 | AAGL |
| ATOM | 1826 | O | ASN | 233 | 25.932 | 33.616 | 124.621 | 1.00 | 34.08 | AAGL |
| ATOM | 1827 | N | LEU | 234 | 24.780 | 34.280 | 122.812 | 1.00 | 32.11 | AAGL |
| ATOM | 1828 | CA | LEU | 234 | 24.331 | 32.927 | 122.498 | 1.00 | 31.75 | AAGL |
| ATOM | 1829 | CB | LEU | 234 | 23.387 | 32.935 | 121.286 | 1.00 | 29.34 | AAGL |
| ATOM | 1830 | CG | LEU | 234 | 21.875 | 33.038 | 121.527 | 1.00 | 28.94 | AAGL |
| ATOM | 1831 | CD1 | LEU | 234 | 21.151 | 33.301 | 120.209 | 1.00 | 28.45 | AAGL |
| ATOM | 1832 | CD2 | LEU | 234 | 21.373 | 31.739 | 122.157 | 1.00 | 29.20 | AAGL |
| ATOM | 1833 | C | LEU | 234 | 25.529 | 32.036 | 122.200 | 1.00 | 31.64 | AAGL |
| ATOM | 1834 | O | LEU | 234 | 25.651 | 30.937 | 122.737 | 1.00 | 31.64 | AAGL |
| ATOM | 1835 | N | GLN | 235 | 26.413 | 32.530 | 121.340 | 1.00 | 31.31 | AAGL |
| ATOM | 1836 | CA | GLN | 235 | 27.601 | 31.797 | 120.944 | 1.00 | 34.83 | AAGL |
| ATOM | 1837 | CB | GLN | 235 | 28.302 | 32.560 | 119.810 | 1.00 | 34.48 | AAGL |
| ATOM | 1838 | CG | GLN | 235 | 29.283 | 31.756 | 118.991 | 1.00 | 36.34 | AAGL |
| ATOM | 1839 | CD | GLN | 235 | 30.545 | 31.410 | 119.747 | 1.00 | 38.22 | AAGL |
| ATOM | 1840 | OE1 | GLN | 235 | 31.065 | 32.224 | 120.511 | 1.00 | 38.29 | AAGL |
| ATOM | 1841 | NE2 | GLN | 235 | 31.059 | 30.204 | 119.521 | 1.00 | 38.94 | AAGL |
| ATOM | 1842 | C | GLN | 235 | 28.557 | 31.597 | 122.122 | 1.00 | 35.64 | AAGL |
| ATOM | 1843 | O | GLN | 235 | 29.063 | 30.500 | 122.335 | 1.00 | 34.97 | AAGL |
| ATOM | 1844 | N | SER | 236 | 28.776 | 32.659 | 122.894 | 1.00 | 36.91 | AAGL |
| ATOM | 1845 | CA | SER | 236 | 29.694 | 32.626 | 124.034 | 1.00 | 39.04 | AAGL |
| ATOM | 1846 | CB | SER | 236 | 29.942 | 34.056 | 124.552 | 1.00 | 39.04 | AAGL |
| ATOM | 1847 | OG | SER | 236 | 28.764 | 34.620 | 125.122 | 1.00 | 40.94 | AAGL |
| ATOM | 1848 | C | SER | 236 | 29.221 | 31.750 | 125.191 | 1.00 | 39.31 | AAGL |
| ATOM | 1849 | O | SER | 236 | 30.027 | 31.118 | 125.885 | 1.00 | 40.12 | AAGL |
| ATOM | 1850 | N | THR | 237 | 27.913 | 31.703 | 125.394 | 1.00 | 38.31 | AAGL |
| ATOM | 1851 | CA | THR | 237 | 27.353 | 30.930 | 126.489 | 1.00 | 37.56 | AAGL |
| ATOM | 1852 | CB | THR | 237 | 26.002 | 31.514 | 126.918 | 1.00 | 36.05 | AAGL |
| ATOM | 1853 | OG1 | THR | 237 | 26.183 | 32.883 | 127.291 | 1.00 | 35.25 | AAGL |
| ATOM | 1854 | CG2 | THR | 237 | 25.432 | 30.738 | 128.101 | 1.00 | 36.50 | AAGL |
| ATOM | 1855 | C | THR | 237 | 27.169 | 29.459 | 126.181 | 1.00 | 36.88 | AAGL |
| ATOM | 1856 | O | THR | 237 | 27.503 | 28.606 | 127.003 | 1.00 | 37.95 | AAGL |
| ATOM | 1857 | N | TYR | 238 | 26.653 | 29.158 | 124.992 | 1.00 | 35.86 | AAGL |
| ATOM | 1858 | CA | TYR | 238 | 26.391 | 27.777 | 124.594 | 1.00 | 34.18 | AAGL |
| ATOM | 1859 | CB | TYR | 238 | 24.955 | 27.684 | 124.059 | 1.00 | 33.21 | AAGL |
| ATOM | 1860 | CG | TYR | 238 | 23.924 | 28.178 | 125.056 | 1.00 | 32.37 | AAGL |
| ATOM | 1861 | CD1 | TYR | 238 | 23.513 | 27.376 | 126.125 | 1.00 | 31.26 | AAGL |
| ATOM | 1862 | CE1 | TYR | 238 | 22.630 | 27.860 | 127.093 | 1.00 | 32.64 | AAGL |
| ATOM | 1863 | CD2 | TYR | 238 | 23.416 | 29.473 | 124.976 | 1.00 | 31.04 | AAGL |
| ATOM | 1864 | CE2 | TYR | 238 | 22.531 | 29.961 | 125.935 | 1.00 | 32.31 | AAGL |

## Fig. 3 cont.

| ATOM | 1865 | CZ | TYR | 238 | 22.146 | 29.150 | 126.992 | 1.00 | 32.31 | AAGL |
|------|------|------|-----|-----|--------|--------|---------|------|-------|------|
| ATOM | 1866 | OH | TYR | 238 | 21.291 | 29.646 | 127.951 | 1.00 | 34.51 | AAGL |
| ATOM | 1867 | C | TYR | 238 | 27.377 | 27.210 | 123.570 | 1.00 | 34.17 | AAGL |
| ATOM | 1868 | O | TYR | 238 | 27.327 | 26.023 | 123.245 | 1.00 | 32.44 | AAGL |
| ATOM | 1869 | N | ASP | 239 | 28.263 | 28.060 | 123.060 | 1.00 | 34.59 | AAGL |
| ATOM | 1870 | CA | ASP | 239 | 29.267 | 27.645 | 122.080 | 1.00 | 35.46 | AAGL |
| ATOM | 1871 | CB | ASP | 239 | 30.292 | 26.716 | 122.754 | 1.00 | 38.30 | AAGL |
| ATOM | 1872 | CG | ASP | 239 | 31.412 | 26.290 | 121.819 | 1.00 | 39.89 | AAGL |
| ATOM | 1873 | OD1 | ASP | 239 | 31.811 | 27.088 | 120.939 | 1.00 | 40.54 | AAGL |
| ATOM | 1874 | OD2 | ASP | 239 | 31.911 | 25.155 | 121.975 | 1.00 | 41.25 | AAGL |
| ATOM | 1875 | C | ASP | 239 | 28.688 | 26.982 | 120.829 | 1.00 | 34.34 | AAGL |
| ATOM | 1876 | O | ASP | 239 | 29.098 | 25.885 | 120.451 | 1.00 | 34.85 | AAGL |
| ATOM | 1877 | N | LYS | 240 | 27.735 | 27.656 | 120.190 | 1.00 | 32.57 | AAGL |
| ATOM | 1878 | CA | LYS | 240 | 27.121 | 27.155 | 118.963 | 1.00 | 31.63 | AAGL |
| ATOM | 1879 | CB | LYS | 240 | 25.746 | 26.525 | 119.234 | 1.00 | 30.18 | AAGL |
| ATOM | 1880 | CG | LYS | 240 | 25.764 | 25.264 | 120.104 | 1.00 | 33.39 | AAGL |
| ATOM | 1881 | CD | LYS | 240 | 24.367 | 24.648 | 120.218 | 1.00 | 31.95 | AAGL |
| ATOM | 1882 | CE | LYS | 240 | 24.318 | 23.502 | 121.247 | 1.00 | 32.26 | AAGL |
| ATOM | 1883 | NZ | LYS | 240 | 25.241 | 22.379 | 120.930 | 1.00 | 29.98 | AAGL |
| ATOM | 1884 | C | LYS | 240 | 26.953 | 28.315 | 117.990 | 1.00 | 29.66 | AAGL |
| ATOM | 1885 | O | LYS | 240 | 26.779 | 29.460 | 118.400 | 1.00 | 30.38 | AAGL |
| ATOM | 1886 | N | PRO | 241 | 27.010 | 28.036 | 116.679 | 1.00 | 29.06 | AAGL |
| ATOM | 1887 | CD | PRO | 241 | 27.422 | 26.781 | 116.028 | 1.00 | 29.36 | AAGL |
| ATOM | 1888 | CA | PRO | 241 | 26.850 | 29.106 | 115.691 | 1.00 | 27.35 | AAGL |
| ATOM | 1889 | CB | PRO | 241 | 27.136 | 28.403 | 114.371 | 1.00 | 27.28 | AAGL |
| ATOM | 1890 | CG | PRO | 241 | 28.058 | 27.285 | 114.768 | 1.00 | 29.28 | AAGL |
| ATOM | 1891 | C | PRO | 241 | 25.434 | 29.693 | 115.732 | 1.00 | 28.09 | AAGL |
| ATOM | 1892 | O | PRO | 241 | 24.491 | 29.048 | 116.201 | 1.00 | 27.43 | AAGL |
| ATOM | 1893 | N | VAL | 242 | 25.294 | 30.911 | 115.225 | 1.00 | 27.44 | AAGL |
| ATOM | 1894 | CA | VAL | 242 | 24.005 | 31.588 | 115.192 | 1.00 | 27.37 | AAGL |
| ATOM | 1895 | CB | VAL | 242 | 24.047 | 32.871 | 116.015 | 1.00 | 24.62 | AAGL |
| ATOM | 1896 | CG1 | VAL | 242 | 24.156 | 32.531 | 117.479 | 1.00 | 27.77 | AAGL |
| ATOM | 1897 | CG2 | VAL | 242 | 25.242 | 33.719 | 115.588 | 1.00 | 27.66 | AAGL |
| ATOM | 1898 | C | VAL | 242 | 23.614 | 31.929 | 113.763 | 1.00 | 26.08 | AAGL |
| ATOM | 1899 | O | VAL | 242 | 24.468 | 32.140 | 112.903 | 1.00 | 27.26 | AAGL |
| ATOM | 1900 | N | VAL | 243 | 22.313 | 31.990 | 113.512 | 1.00 | 25.38 | AAGL |
| ATOM | 1901 | CA | VAL | 243 | 21.806 | 32.287 | 112.179 | 1.00 | 22.94 | AAGL |
| ATOM | 1902 | CB | VAL | 243 | 21.431 | 30.973 | 111.419 | 1.00 | 24.38 | AAGL |
| ATOM | 1903 | CG1 | VAL | 243 | 20.994 | 31.285 | 109.996 | 1.00 | 23.02 | AAGL |
| ATOM | 1904 | CG2 | VAL | 243 | 22.612 | 30.009 | 111.409 | 1.00 | 25.53 | AAGL |
| ATOM | 1905 | C | VAL | 243 | 20.541 | 33.129 | 112.289 | 1.00 | 22.55 | AAGL |
| ATOM | 1906 | O | VAL | 243 | 19.691 | 32.836 | 113.115 | 1.00 | 21.01 | AAGL |
| ATOM | 1907 | N | VAL | 244 | 20.432 | 34.188 | 111.487 | 1.00 | 21.40 | AAGL |
| ATOM | 1908 | CA | VAL | 244 | 19.213 | 34.995 | 111.483 | 1.00 | 21.25 | AAGL |
| ATOM | 1909 | CB | VAL | 244 | 19.469 | 36.463 | 111.094 | 1.00 | 21.49 | AAGL |
| ATOM | 1910 | CG1 | VAL | 244 | 18.139 | 37.170 | 110.884 | 1.00 | 22.74 | AAGL |
| ATOM | 1911 | CG2 | VAL | 244 | 20.263 | 37.163 | 112.188 | 1.00 | 20.20 | AAGL |
| ATOM | 1912 | C | VAL | 244 | 18.414 | 34.309 | 110.387 | 1.00 | 19.60 | AAGL |
| ATOM | 1913 | O | VAL | 244 | 18.720 | 34.446 | 109.205 | 1.00 | 20.42 | AAGL |
| ATOM | 1914 | N | VAL | 245 | 17.395 | 33.557 | 110.780 | 1.00 | 17.97 | AAGL |
| ATOM | 1915 | CA | VAL | 245 | 16.635 | 32.788 | 109.807 | 1.00 | 17.90 | AAGL |
| ATOM | 1916 | CB | VAL | 245 | 16.234 | 31.431 | 110.413 | 1.00 | 18.93 | AAGL |
| ATOM | 1917 | CG1 | VAL | 245 | 17.485 | 30.699 | 110.871 | 1.00 | 18.12 | AAGL |
| ATOM | 1918 | CG2 | VAL | 245 | 15.274 | 31.637 | 111.578 | 1.00 | 17.48 | AAGL |
| ATOM | 1919 | C | VAL | 245 | 15.415 | 33.450 | 109.192 | 1.00 | 17.32 | AAGL |
| ATOM | 1920 | O | VAL | 245 | 14.783 | 32.882 | 108.308 | 1.00 | 17.57 | AAGL |
| ATOM | 1921 | N | GLU | 246 | 15.085 | 34.644 | 109.666 | 1.00 | 17.88 | AAGL |
| ATOM | 1922 | CA | GLU | 246 | 13.949 | 35.392 | 109.143 | 1.00 | 18.02 | AAGL |
| ATOM | 1923 | CB | GLU | 246 | 12.657 | 35.023 | 109.875 | 1.00 | 22.04 | AAGL |
| ATOM | 1924 | CG | GLU | 246 | 11.917 | 33.816 | 109.352 | 1.00 | 22.72 | AAGL |
| ATOM | 1925 | CD | GLU | 246 | 10.611 | 33.589 | 110.102 | 1.00 | 24.03 | AAGL |
| ATOM | 1926 | OE1 | GLU | 246 | 9.882 | 34.579 | 110.340 | 1.00 | 20.71 | AAGL |
| ATOM | 1927 | OE2 | GLU | 246 | 10.311 | 32.422 | 110.438 | 1.00 | 22.70 | AAGL |
| ATOM | 1928 | C | GLU | 246 | 14.163 | 36.882 | 109.327 | 1.00 | 18.20 | AAGL |
| ATOM | 1929 | O | GLU | 246 | 14.547 | 37.316 | 110.404 | 1.00 | 19.12 | AAGL |
| ATOM | 1930 | N | THR | 247 | 13.912 | 37.658 | 108.281 | 1.00 | 17.83 | AAGL |
| ATOM | 1931 | CA | THR | 247 | 14.024 | 39.114 | 108.372 | 1.00 | 19.34 | AAGL |

# Fig. 3 cont.

| ATOM | 1932 | CB | THR | 247 | 15.505 | 39.584 | 108.487 | 1.00 | 21.29 | AAGL |
|------|------|-----|-----|-----|--------|--------|---------|------|-------|------|
| ATOM | 1933 | OG1 | THR | 247 | 15.532 | 40.968 | 108.857 | 1.00 | 22.65 | AAGL |
| ATOM | 1934 | CG2 | THR | 247 | 16.238 | 39.409 | 107.172 | 1.00 | 20.07 | AAGL |
| ATOM | 1935 | C | THR | 247 | 13.356 | 39.774 | 107.167 | 1.00 | 18.87 | AAGL |
| ATOM | 1936 | O | THR | 247 | 13.167 | 39.141 | 106.134 | 1.00 | 19.64 | AAGL |
| ATOM | 1937 | N | ASN | 248 | 12.980 | 41.039 | 107.326 | 1.00 | 17.13 | AAGL |
| ATOM | 1938 | CA | ASN | 248 | 12.312 | 41.816 | 106.281 | 1.00 | 18.39 | AAGL |
| ATOM | 1939 | CB | ASN | 248 | 10.793 | 41.800 | 106.466 | 1.00 | 19.04 | AAGL |
| ATOM | 1940 | CG | ASN | 248 | 10.095 | 40.616 | 105.836 | 1.00 | 20.07 | AAGL |
| ATOM | 1941 | OD1 | ASN | 248 | 8.889 | 40.475 | 106.007 | 1.00 | 23.76 | AAGL |
| ATOM | 1942 | ND2 | ASN | 248 | 10.820 | 39.775 | 105.113 | 1.00 | 20.10 | AAGL |
| ATOM | 1943 | C | ASN | 248 | 12.685 | 43.291 | 106.427 | 1.00 | 18.69 | AAGL |
| ATOM | 1944 | O | ASN | 248 | 13.135 | 43.725 | 107.483 | 1.00 | 17.33 | AAGL |
| ATOM | 1945 | N | TRP | 249 | 12.466 | 44.046 | 105.355 | 1.00 | 19.91 | AAGL |
| ATOM | 1946 | CA | TRP | 249 | 12.630 | 45.503 | 105.355 | 1.00 | 21.18 | AAGL |
| ATOM | 1947 | CB | TRP | 249 | 14.065 | 45.981 | 105.129 | 1.00 | 21.42 | AAGL |
| ATOM | 1948 | CG | TRP | 249 | 14.117 | 47.491 | 105.288 | 1.00 | 19.99 | AAGL |
| ATOM | 1949 | CD2 | TRP | 249 | 14.261 | 48.225 | 106.517 | 1.00 | 19.73 | AAGL |
| ATOM | 1950 | CE2 | TRP | 249 | 14.108 | 49.599 | 106.208 | 1.00 | 19.65 | AAGL |
| ATOM | 1951 | CE3 | TRP | 249 | 14.499 | 47.853 | 107.847 | 1.00 | 19.37 | AAGL |
| ATOM | 1952 | CD1 | TRP | 249 | 13.895 | 48.431 | 104.313 | 1.00 | 20.84 | AAGL |
| ATOM | 1953 | NE1 | TRP | 249 | 13.887 | 49.693 | 104.861 | 1.00 | 19.99 | AAGL |
| ATOM | 1954 | CZ2 | TRP | 249 | 14.185 | 50.604 | 107.187 | 1.00 | 20.08 | AAGL |
| ATOM | 1955 | CZ3 | TRP | 249 | 14.575 | 48.853 | 108.820 | 1.00 | 21.35 | AAGL |
| ATOM | 1956 | CH2 | TRP | 249 | 14.418 | 50.214 | 108.481 | 1.00 | 21.66 | AAGL |
| ATOM | 1957 | C | TRP | 249 | 11.722 | 46.003 | 104.241 | 1.00 | 20.70 | AAGL |
| ATOM | 1958 | O | TRP | 249 | 11.800 | 45.539 | 103.102 | 1.00 | 22.36 | AAGL |
| ATOM | 1959 | N | PRO | 250 | 10.838 | 46.957 | 104.559 | 1.00 | 22.00 | AAGL |
| ATOM | 1960 | CD | PRO | 250 | 10.686 | 47.625 | 105.865 | 1.00 | 21.04 | AAGL |
| ATOM | 1961 | CA | PRO | 250 | 9.894 | 47.508 | 103.587 | 1.00 | 21.27 | AAGL |
| ATOM | 1962 | CB | PRO | 250 | 8.876 | 48.210 | 104.477 | 1.00 | 22.31 | AAGL |
| ATOM | 1963 | CG | PRO | 250 | 9.744 | 48.783 | 105.538 | 1.00 | 22.64 | AAGL |
| ATOM | 1964 | C | PRO | 250 | 10.402 | 48.435 | 102.507 | 1.00 | 23.33 | AAGL |
| ATOM | 1965 | O | PRO | 250 | 11.270 | 49.268 | 102.743 | 1.00 | 21.79 | AAGL |
| ATOM | 1966 | N | VAL | 251 | 9.844 | 48.282 | 101.311 | 1.00 | 23.27 | AAGL |
| ATOM | 1967 | CA | VAL | 251 | 10.185 | 49.165 | 100.212 | 1.00 | 24.85 | AAGL |
| ATOM | 1968 | CB | VAL | 251 | 10.171 | 48.437 | 98.854 | 1.00 | 24.44 | AAGL |
| ATOM | 1969 | CG1 | VAL | 251 | 11.335 | 47.476 | 98.787 | 1.00 | 24.31 | AAGL |
| ATOM | 1970 | CG2 | VAL | 251 | 8.865 | 47.699 | 98.657 | 1.00 | 28.76 | AAGL |
| ATOM | 1971 | C | VAL | 251 | 9.095 | 50.227 | 100.278 | 1.00 | 26.42 | AAGL |
| ATOM | 1972 | O | VAL | 251 | 9.177 | 51.281 | 99.646 | 1.00 | 24.68 | AAGL |
| ATOM | 1973 | N | SER | 252 | 8.075 | 49.934 | 101.083 | 1.00 | 27.57 | AAGL |
| ATOM | 1974 | CA | SER | 252 | 6.962 | 50.851 | 101.298 | 1.00 | 27.22 | AAGL |
| ATOM | 1975 | CB | SER | 252 | 5.942 | 50.722 | 100.164 | 1.00 | 28.72 | AAGL |
| ATOM | 1976 | OG | SER | 252 | 4.895 | 51.662 | 100.327 | 1.00 | 28.82 | AAGL |
| ATOM | 1977 | C | SER | 252 | 6.289 | 50.558 | 102.642 | 1.00 | 28.31 | AAGL |
| ATOM | 1978 | O | SER | 252 | 5.858 | 49.434 | 102.886 | 1.00 | 26.39 | AAGL |
| ATOM | 1979 | N | CYS | 253 | 6.232 | 51.559 | 103.518 | 1.00 | 27.82 | AAGL |
| ATOM | 1980 | CA | CYS | 253 | 5.594 | 51.413 | 104.824 | 1.00 | 27.19 | AAGL |
| ATOM | 1981 | C | CYS | 253 | 4.932 | 52.738 | 105.201 | 1.00 | 28.86 | AAGL |
| ATOM | 1982 | O | CYS | 253 | 5.411 | 53.436 | 106.091 | 1.00 | 27.40 | AAGL |
| ATOM | 1983 | CB | CYS | 253 | 6.611 | 51.031 | 105.913 | 1.00 | 27.78 | AAGL |
| ATOM | 1984 | SG | CYS | 253 | 5.803 | 50.369 | 107.406 | 1.00 | 28.15 | AAGL |
| ATOM | 1985 | N | PRO | 254 | 3.812 | 53.089 | 104.528 | 1.00 | 30.47 | AAGL |
| ATOM | 1986 | CD | PRO | 254 | 3.166 | 52.222 | 103.525 | 1.00 | 30.66 | AAGL |
| ATOM | 1987 | CA | PRO | 254 | 3.022 | 54.314 | 104.725 | 1.00 | 32.44 | AAGL |
| ATOM | 1988 | CB | PRO | 254 | 1.739 | 54.023 | 103.951 | 1.00 | 32.43 | AAGL |
| ATOM | 1989 | CG | PRO | 254 | 2.206 | 53.171 | 102.837 | 1.00 | 33.11 | AAGL |
| ATOM | 1990 | C | PRO | 254 | 2.739 | 54.660 | 106.181 | 1.00 | 34.76 | AAGL |
| ATOM | 1991 | O | PRO | 254 | 2.780 | 55.828 | 106.570 | 1.00 | 35.87 | AAGL |
| ATOM | 1992 | N | ASN | 255 | 2.429 | 53.653 | 106.987 | 1.00 | 35.37 | AAGL |
| ATOM | 1993 | CA | ASN | 255 | 2.161 | 53.912 | 108.392 | 1.00 | 36.89 | AAGL |
| ATOM | 1994 | CB | ASN | 255 | 0.755 | 54.457 | 108.575 | 1.00 | 37.41 | AAGL |
| ATOM | 1995 | CG | ASN | 255 | 0.410 | 54.682 | 110.030 | 1.00 | 38.46 | AAGL |
| ATOM | 1996 | OD1 | ASN | 255 | 1.254 | 55.124 | 110.832 | 1.00 | 35.39 | AAGL |
| ATOM | 1997 | ND2 | ASN | 255 | -0.833 | 54.389 | 110.387 | 1.00 | 34.81 | AAGL |
| ATOM | 1998 | C | ASN | 255 | 2.354 | 52.691 | 109.263 | 1.00 | 35.87 | AAGL |

# Fig. 3 cont.

| ATOM | 1999 | O   | ASN | 255 | 1.471  | 51.841 | 109.375 | 1.00 | 36.70 | AAGL |
|------|------|-----|-----|-----|--------|--------|---------|------|-------|------|
| ATOM | 2000 | N   | PRO | 256 | 3.520  | 52.601 | 109.910 | 1.00 | 35.76 | AAGL |
| ATOM | 2001 | CD  | PRO | 256 | 4.640  | 53.550 | 109.780 | 1.00 | 35.85 | AAGL |
| ATOM | 2002 | CA  | PRO | 256 | 3.878  | 51.493 | 110.791 | 1.00 | 34.93 | AAGL |
| ATOM | 2003 | CB  | PRO | 256 | 5.387  | 51.654 | 110.927 | 1.00 | 35.60 | AAGL |
| ATOM | 2004 | CG  | PRO | 256 | 5.558  | 53.122 | 110.901 | 1.00 | 36.37 | AAGL |
| ATOM | 2005 | C   | PRO | 256 | 3.158  | 51.543 | 112.140 | 1.00 | 34.50 | AAGL |
| ATOM | 2006 | O   | PRO | 256 | 3.041  | 52.604 | 112.752 | 1.00 | 33.71 | AAGL |
| ATOM | 2007 | N   | ALA | 257 | 2.683  | 50.393 | 112.603 | 1.00 | 32.93 | AAGL |
| ATOM | 2008 | CA  | ALA | 257 | 1.988  | 50.327 | 113.880 | 1.00 | 31.85 | AAGL |
| ATOM | 2009 | CB  | ALA | 257 | 1.371  | 48.946 | 114.079 | 1.00 | 31.01 | AAGL |
| ATOM | 2010 | C   | ALA | 257 | 2.970  | 50.621 | 115.000 | 1.00 | 32.12 | AAGL |
| ATOM | 2011 | O   | ALA | 257 | 2.591  | 51.139 | 116.046 | 1.00 | 31.82 | AAGL |
| ATOM | 2012 | N   | TYR | 258 | 4.237  | 50.291 | 114.771 | 1.00 | 31.15 | AAGL |
| ATOM | 2013 | CA  | TYR | 258 | 5.279  | 50.504 | 115.761 | 1.00 | 32.72 | AAGL |
| ATOM | 2014 | CB  | TYR | 258 | 5.892  | 49.168 | 116.169 | 1.00 | 35.88 | AAGL |
| ATOM | 2015 | CG  | TYR | 258 | 4.954  | 48.226 | 116.880 | 1.00 | 38.05 | AAGL |
| ATOM | 2016 | CD1 | TYR | 258 | 4.136  | 47.341 | 116.170 | 1.00 | 37.62 | AAGL |
| ATOM | 2017 | CE1 | TYR | 258 | 3.276  | 46.468 | 116.840 | 1.00 | 40.53 | AAGL |
| ATOM | 2018 | CD2 | TYR | 258 | 4.889  | 48.216 | 118.267 | 1.00 | 39.82 | AAGL |
| ATOM | 2019 | CE2 | TYR | 258 | 4.039  | 47.357 | 118.943 | 1.00 | 41.64 | AAGL |
| ATOM | 2020 | CZ  | TYR | 258 | 3.236  | 46.489 | 118.232 | 1.00 | 42.48 | AAGL |
| ATOM | 2021 | OH  | TYR | 258 | 2.386  | 45.659 | 118.934 | 1.00 | 45.83 | AAGL |
| ATOM | 2022 | C   | TYR | 258 | 6.414  | 51.411 | 115.293 | 1.00 | 32.44 | AAGL |
| ATOM | 2023 | O   | TYR | 258 | 6.736  | 51.468 | 114.108 | 1.00 | 31.27 | AAGL |
| ATOM | 2024 | N   | ALA | 259 | 7.021  | 52.121 | 116.237 | 1.00 | 30.79 | AAGL |
| ATOM | 2025 | CA  | ALA | 259 | 8.147  | 52.983 | 115.919 | 1.00 | 31.35 | AAGL |
| ATOM | 2026 | CB  | ALA | 259 | 8.479  | 53.864 | 117.118 | 1.00 | 33.39 | AAGL |
| ATOM | 2027 | C   | ALA | 259 | 9.315  | 52.046 | 115.607 | 1.00 | 29.93 | AAGL |
| ATOM | 2028 | O   | ALA | 259 | 9.458  | 51.004 | 116.242 | 1.00 | 29.16 | AAGL |
| ATOM | 2029 | N   | PHE | 260 | 10.137 | 52.392 | 114.623 | 1.00 | 29.81 | AAGL |
| ATOM | 2030 | CA  | PHE | 260 | 11.281 | 51.548 | 114.285 | 1.00 | 29.03 | AAGL |
| ATOM | 2031 | CB  | PHE | 260 | 11.772 | 51.871 | 112.867 | 1.00 | 28.71 | AAGL |
| ATOM | 2032 | CG  | PHE | 260 | 11.007 | 51.157 | 111.776 | 1.00 | 29.00 | AAGL |
| ATOM | 2033 | CD1 | PHE | 260 | 9.622  | 51.242 | 111.704 | 1.00 | 29.61 | AAGL |
| ATOM | 2034 | CD2 | PHE | 260 | 11.676 | 50.379 | 110.840 | 1.00 | 28.02 | AAGL |
| ATOM | 2035 | CE1 | PHE | 260 | 8.915  | 50.558 | 110.720 | 1.00 | 30.59 | AAGL |
| ATOM | 2036 | CE2 | PHE | 260 | 10.979 | 49.694 | 109.854 | 1.00 | 29.46 | AAGL |
| ATOM | 2037 | CZ  | PHE | 260 | 9.594  | 49.783 | 109.796 | 1.00 | 29.30 | AAGL |
| ATOM | 2038 | C   | PHE | 260 | 12.409 | 51.765 | 115.300 | 1.00 | 29.23 | AAGL |
| ATOM | 2039 | O   | PHE | 260 | 12.464 | 52.806 | 115.957 | 1.00 | 29.38 | AAGL |
| ATOM | 2040 | N   | PRO | 261 | 13.302 | 50.771 | 115.466 | 1.00 | 29.34 | AAGL |
| ATOM | 2041 | CD  | PRO | 261 | 13.247 | 49.414 | 114.891 | 1.00 | 29.47 | AAGL |
| ATOM | 2042 | CA  | PRO | 261 | 14.418 | 50.891 | 116.409 | 1.00 | 29.63 | AAGL |
| ATOM | 2043 | CB  | PRO | 261 | 15.194 | 49.599 | 116.186 | 1.00 | 28.18 | AAGL |
| ATOM | 2044 | CG  | PRO | 261 | 14.096 | 48.617 | 115.852 | 1.00 | 28.51 | AAGL |
| ATOM | 2045 | C   | PRO | 261 | 15.240 | 52.137 | 116.063 | 1.00 | 29.95 | AAGL |
| ATOM | 2046 | O   | PRO | 261 | 15.312 | 52.539 | 114.897 | 1.00 | 30.37 | AAGL |
| ATOM | 2047 | N   | SER | 262 | 15.846 | 52.736 | 117.082 | 1.00 | 32.41 | AAGL |
| ATOM | 2048 | CA  | SER | 262 | 16.637 | 53.951 | 116.922 | 1.00 | 31.88 | AAGL |
| ATOM | 2049 | CB  | SER | 262 | 17.167 | 54.396 | 118.291 | 1.00 | 33.67 | AAGL |
| ATOM | 2050 | OG  | SER | 262 | 17.708 | 53.295 | 119.003 | 1.00 | 37.49 | AAGL |
| ATOM | 2051 | C   | SER | 262 | 17.785 | 53.858 | 115.918 | 1.00 | 32.30 | AAGL |
| ATOM | 2052 | O   | SER | 262 | 17.967 | 54.773 | 115.107 | 1.00 | 32.95 | AAGL |
| ATOM | 2053 | N   | ASP | 263 | 18.565 | 52.778 | 115.955 | 1.00 | 31.17 | AAGL |
| ATOM | 2054 | CA  | ASP | 263 | 19.660 | 52.663 | 115.000 | 1.00 | 31.60 | AAGL |
| ATOM | 2055 | CB  | ASP | 263 | 20.768 | 51.724 | 115.512 | 1.00 | 31.48 | AAGL |
| ATOM | 2056 | CG  | ASP | 263 | 20.241 | 50.418 | 116.090 | 1.00 | 31.74 | AAGL |
| ATOM | 2057 | OD1 | ASP | 263 | 19.111 | 49.994 | 115.748 | 1.00 | 30.33 | AAGL |
| ATOM | 2058 | OD2 | ASP | 263 | 20.987 | 49.796 | 116.887 | 1.00 | 30.41 | AAGL |
| ATOM | 2059 | C   | ASP | 263 | 19.210 | 52.227 | 113.604 | 1.00 | 31.45 | AAGL |
| ATOM | 2060 | O   | ASP | 263 | 20.036 | 51.858 | 112.768 | 1.00 | 32.04 | AAGL |
| ATOM | 2061 | N   | LEU | 264 | 17.905 | 52.296 | 113.344 | 1.00 | 30.59 | AAGL |
| ATOM | 2062 | CA  | LEU | 264 | 17.363 | 51.920 | 112.038 | 1.00 | 28.75 | AAGL |
| ATOM | 2063 | CB  | LEU | 264 | 16.621 | 50.575 | 112.123 | 1.00 | 27.83 | AAGL |
| ATOM | 2064 | CG  | LEU | 264 | 17.375 | 49.323 | 112.570 | 1.00 | 24.26 | AAGL |
| ATOM | 2065 | CD1 | LEU | 264 | 16.389 | 48.179 | 112.752 | 1.00 | 25.96 | AAGL |

# Fig. 3 cont.

| ATOM | 2066 | CD2  | LEU | 264 | 18.429 | 48.955 | 111.552 | 1.00 | 27.53 | AAGL |
|------|------|------|-----|-----|--------|--------|---------|------|-------|------|
| ATOM | 2067 | C    | LEU | 264 | 16.391 | 52.971 | 111.512 | 1.00 | 28.95 | AAGL |
| ATOM | 2068 | O    | LEU | 264 | 15.941 | 52.893 | 110.374 | 1.00 | 27.43 | AAGL |
| ATOM | 2069 | N    | SER | 265 | 16.074 | 53.965 | 112.331 | 1.00 | 30.75 | AAGL |
| ATOM | 2070 | CA   | SER | 265 | 15.120 | 54.986 | 111.925 | 1.00 | 32.24 | AAGL |
| ATOM | 2071 | CB   | SER | 265 | 14.662 | 55.779 | 113.154 | 1.00 | 33.67 | AAGL |
| ATOM | 2072 | OG   | SER | 265 | 15.763 | 56.287 | 113.892 | 1.00 | 34.70 | AAGL |
| ATOM | 2073 | C    | SER | 265 | 15.572 | 55.941 | 110.815 | 1.00 | 33.25 | AAGL |
| ATOM | 2074 | O    | SER | 265 | 14.776 | 56.742 | 110.328 | 1.00 | 34.94 | AAGL |
| ATOM | 2075 | N    | SER | 266 | 16.832 | 55.859 | 110.399 | 1.00 | 33.96 | AAGL |
| ATOM | 2076 | CA   | SER | 266 | 17.305 | 56.745 | 109.339 | 1.00 | 33.28 | AAGL |
| ATOM | 2077 | CB   | SER | 266 | 18.765 | 57.133 | 109.576 | 1.00 | 34.74 | AAGL |
| ATOM | 2078 | OG   | SER | 266 | 19.652 | 56.107 | 109.142 | 1.00 | 40.32 | AAGL |
| ATOM | 2079 | C    | SER | 266 | 17.176 | 56.085 | 107.964 | 1.00 | 31.87 | AAGL |
| ATOM | 2080 | O    | SER | 266 | 17.236 | 56.754 | 106.931 | 1.00 | 30.82 | AAGL |
| ATOM | 2081 | N    | ILE | 267 | 16.982 | 54.773 | 107.956 | 1.00 | 28.10 | AAGL |
| ATOM | 2082 | CA   | ILE | 267 | 16.874 | 54.025 | 106.713 | 1.00 | 26.55 | AAGL |
| ATOM | 2083 | CB   | ILE | 267 | 17.067 | 52.523 | 106.983 | 1.00 | 25.69 | AAGL |
| ATOM | 2084 | CG2  | ILE | 267 | 17.120 | 51.757 | 105.666 | 1.00 | 26.74 | AAGL |
| ATOM | 2085 | CG1  | ILE | 267 | 18.349 | 52.323 | 107.801 | 1.00 | 28.70 | AAGL |
| ATOM | 2086 | CD1  | ILE | 267 | 18.606 | 50.889 | 108.250 | 1.00 | 27.91 | AAGL |
| ATOM | 2087 | C    | ILE | 267 | 15.537 | 54.267 | 106.024 | 1.00 | 25.54 | AAGL |
| ATOM | 2088 | O    | ILE | 267 | 14.482 | 54.060 | 106.604 | 1.00 | 24.26 | AAGL |
| ATOM | 2089 | N    | PRO | 268 | 15.567 | 54.734 | 104.767 | 1.00 | 25.09 | AAGL |
| ATOM | 2090 | CD   | PRO | 268 | 16.725 | 55.097 | 103.932 | 1.00 | 26.35 | AAGL |
| ATOM | 2091 | CA   | PRO | 268 | 14.312 | 54.986 | 104.058 | 1.00 | 25.07 | AAGL |
| ATOM | 2092 | CB   | PRO | 268 | 14.767 | 55.792 | 102.844 | 1.00 | 26.89 | AAGL |
| ATOM | 2093 | CG   | PRO | 268 | 16.108 | 55.205 | 102.560 | 1.00 | 26.87 | AAGL |
| ATOM | 2094 | C    | PRO | 268 | 13.602 | 53.694 | 103.662 | 1.00 | 24.21 | AAGL |
| ATOM | 2095 | O    | PRO | 268 | 14.208 | 52.622 | 103.644 | 1.00 | 23.10 | AAGL |
| ATOM | 2096 | N    | PHE | 269 | 12.313 | 53.806 | 103.362 | 1.00 | 23.20 | AAGL |
| ATOM | 2097 | CA   | PHE | 269 | 11.525 | 52.664 | 102.931 | 1.00 | 23.46 | AAGL |
| ATOM | 2098 | CB   | PHE | 269 | 10.091 | 52.765 | 103.446 | 1.00 | 24.32 | AAGL |
| ATOM | 2099 | CG   | PHE | 269 | 9.994  | 52.861 | 104.942 | 1.00 | 24.64 | AAGL |
| ATOM | 2100 | CD1  | PHE | 269 | 10.819 | 52.093 | 105.758 | 1.00 | 25.88 | AAGL |
| ATOM | 2101 | CD2  | PHE | 269 | 9.070  | 53.706 | 105.535 | 1.00 | 25.95 | AAGL |
| ATOM | 2102 | CE1  | PHE | 269 | 10.722 | 52.168 | 107.151 | 1.00 | 26.08 | AAGL |
| ATOM | 2103 | CE2  | PHE | 269 | 8.965  | 53.788 | 106.925 | 1.00 | 23.79 | AAGL |
| ATOM | 2104 | CZ   | PHE | 269 | 9.793  | 53.016 | 107.732 | 1.00 | 23.02 | AAGL |
| ATOM | 2105 | C    | PHE | 269 | 11.548 | 52.698 | 101.413 | 1.00 | 23.22 | AAGL |
| ATOM | 2106 | O    | PHE | 269 | 10.778 | 53.420 | 100.774 | 1.00 | 23.95 | AAGL |
| ATOM | 2107 | N    | SER | 270 | 12.462 | 51.916 | 100.848 | 1.00 | 23.29 | AAGL |
| ATOM | 2108 | CA   | SER | 270 | 12.649 | 51.848 | 99.410  | 1.00 | 24.41 | AAGL |
| ATOM | 2109 | CB   | SER | 270 | 13.282 | 53.140 | 98.924  | 1.00 | 24.90 | AAGL |
| ATOM | 2110 | OG   | SER | 270 | 14.547 | 53.300 | 99.540  | 1.00 | 25.23 | AAGL |
| ATOM | 2111 | C    | SER | 270 | 13.596 | 50.702 | 99.125  | 1.00 | 22.81 | AAGL |
| ATOM | 2112 | O    | SER | 270 | 14.147 | 50.105 | 100.055 | 1.00 | 25.01 | AAGL |
| ATOM | 2113 | N    | VAL | 271 | 13.791 | 50.392 | 97.845  | 1.00 | 23.71 | AAGL |
| ATOM | 2114 | CA   | VAL | 271 | 14.702 | 49.316 | 97.477  | 1.00 | 22.85 | AAGL |
| ATOM | 2115 | CB   | VAL | 271 | 14.846 | 49.170 | 95.948  | 1.00 | 24.85 | AAGL |
| ATOM | 2116 | CG1  | VAL | 271 | 15.953 | 48.172 | 95.630  | 1.00 | 23.46 | AAGL |
| ATOM | 2117 | CG2  | VAL | 271 | 13.534 | 48.698 | 95.338  | 1.00 | 22.67 | AAGL |
| ATOM | 2118 | C    | VAL | 271 | 16.065 | 49.649 | 98.056  | 1.00 | 24.60 | AAGL |
| ATOM | 2119 | O    | VAL | 271 | 16.744 | 48.787 | 98.613  | 1.00 | 24.45 | AAGL |
| ATOM | 2120 | N    | ALA | 272 | 16.453 | 50.914 | 97.932  | 1.00 | 25.33 | AAGL |
| ATOM | 2121 | CA   | ALA | 272 | 17.740 | 51.373 | 98.442  | 1.00 | 24.59 | AAGL |
| ATOM | 2122 | CB   | ALA | 272 | 17.946 | 52.858 | 98.104  | 1.00 | 26.33 | AAGL |
| ATOM | 2123 | C    | ALA | 272 | 17.814 | 51.162 | 99.951  | 1.00 | 21.83 | AAGL |
| ATOM | 2124 | O    | ALA | 272 | 18.839 | 50.732 | 100.479 | 1.00 | 21.37 | AAGL |
| ATOM | 2125 | N    | GLY | 273 | 16.722 | 51.463 | 100.646 | 1.00 | 22.29 | AAGL |
| ATOM | 2126 | CA   | GLY | 273 | 16.710 | 51.284 | 102.086 | 1.00 | 22.02 | AAGL |
| ATOM | 2127 | C    | GLY | 273 | 16.808 | 49.814 | 102.448 | 1.00 | 21.98 | AAGL |
| ATOM | 2128 | O    | GLY | 273 | 17.427 | 49.442 | 103.443 | 1.00 | 22.94 | AAGL |
| ATOM | 2129 | N    | GLN | 274 | 16.192 | 48.973 | 101.623 | 1.00 | 23.13 | AAGL |
| ATOM | 2130 | CA   | GLN | 274 | 16.210 | 47.534 | 101.837 | 1.00 | 23.82 | AAGL |
| ATOM | 2131 | CB   | GLN | 274 | 15.354 | 46.862 | 100.770 | 1.00 | 26.47 | AAGL |
| ATOM | 2132 | CG   | GLN | 274 | 14.976 | 45.429 | 101.049 | 1.00 | 28.49 | AAGL |

# Fig. 3 cont.

| ATOM | 2133 | CD | GLN | 274 | 13.969 | 44.926 | 100.034 | 1.00 | 29.11 | AAGL |
|------|------|------|-----|-----|--------|--------|---------|------|-------|------|
| ATOM | 2134 | OE1 | GLN | 274 | 14.273 | 44.819 | 98.846 | 1.00 | 26.58 | AAGL |
| ATOM | 2135 | NE2 | GLN | 274 | 12.760 | 44.630 | 100.491 | 1.00 | 22.87 | AAGL |
| ATOM | 2136 | C | GLN | 274 | 17.655 | 47.047 | 101.741 | 1.00 | 24.42 | AAGL |
| ATOM | 2137 | O | GLN | 274 | 18.090 | 46.184 | 102.500 | 1.00 | 23.54 | AAGL |
| ATOM | 2138 | N | GLN | 275 | 18.405 | 47.621 | 100.807 | 1.00 | 22.92 | AAGL |
| ATOM | 2139 | CA | GLN | 275 | 19.802 | 47.240 | 100.627 | 1.00 | 22.23 | AAGL |
| ATOM | 2140 | CB | GLN | 275 | 20.347 | 47.863 | 99.349 | 1.00 | 25.17 | AAGL |
| ATOM | 2141 | CG | GLN | 275 | 19.668 | 47.370 | 98.089 | 1.00 | 25.16 | AAGL |
| ATOM | 2142 | CD | GLN | 275 | 20.162 | 48.099 | 96.862 | 1.00 | 29.65 | AAGL |
| ATOM | 2143 | OE1 | GLN | 275 | 19.879 | 49.283 | 96.677 | 1.00 | 33.06 | AAGL |
| ATOM | 2144 | NE2 | GLN | 275 | 20.915 | 47.403 | 96.021 | 1.00 | 30.34 | AAGL |
| ATOM | 2145 | C | GLN | 275 | 20.658 | 47.679 | 101.807 | 1.00 | 22.46 | AAGL |
| ATOM | 2146 | O | GLN | 275 | 21.492 | 46.924 | 102.289 | 1.00 | 23.14 | AAGL |
| ATOM | 2147 | N | GLU | 276 | 20.444 | 48.906 | 102.268 | 1.00 | 23.39 | AAGL |
| ATOM | 2148 | CA | GLU | 276 | 21.203 | 49.448 | 103.386 | 1.00 | 22.93 | AAGL |
| ATOM | 2149 | CB | GLU | 276 | 20.821 | 50.917 | 103.615 | 1.00 | 26.77 | AAGL |
| ATOM | 2150 | CG | GLU | 276 | 21.393 | 51.518 | 104.891 | 1.00 | 31.09 | AAGL |
| ATOM | 2151 | CD | GLU | 276 | 21.007 | 52.982 | 105.081 | 1.00 | 33.52 | AAGL |
| ATOM | 2152 | OE1 | GLU | 276 | 19.968 | 53.402 | 104.533 | 1.00 | 35.95 | AAGL |
| ATOM | 2153 | OE2 | GLU | 276 | 21.734 | 53.704 | 105.791 | 1.00 | 34.45 | AAGL |
| ATOM | 2154 | C | GLU | 276 | 20.948 | 48.620 | 104.643 | 1.00 | 23.86 | AAGL |
| ATOM | 2155 | O | GLU | 276 | 21.870 | 48.302 | 105.385 | 1.00 | 22.86 | AAGL |
| ATOM | 2156 | N | PHE | 277 | 19.692 | 48.261 | 104.876 | 1.00 | 22.41 | AAGL |
| ATOM | 2157 | CA | PHE | 277 | 19.355 | 47.458 | 106.042 | 1.00 | 21.05 | AAGL |
| ATOM | 2158 | CB | PHE | 277 | 17.844 | 47.222 | 106.120 | 1.00 | 20.89 | AAGL |
| ATOM | 2159 | CG | PHE | 277 | 17.447 | 46.219 | 107.171 | 1.00 | 19.02 | AAGL |
| ATOM | 2160 | CD1 | PHE | 277 | 17.541 | 46.533 | 108.518 | 1.00 | 21.55 | AAGL |
| ATOM | 2161 | CD2 | PHE | 277 | 17.003 | 44.946 | 106.805 | 1.00 | 22.72 | AAGL |
| ATOM | 2162 | CE1 | PHE | 277 | 17.200 | 45.594 | 109.498 | 1.00 | 23.87 | AAGL |
| ATOM | 2163 | CE2 | PHE | 277 | 16.660 | 43.998 | 107.781 | 1.00 | 21.01 | AAGL |
| ATOM | 2164 | CZ | PHE | 277 | 16.759 | 44.323 | 109.122 | 1.00 | 22.10 | AAGL |
| ATOM | 2165 | C | PHE | 277 | 20.051 | 46.102 | 105.989 | 1.00 | 20.46 | AAGL |
| ATOM | 2166 | O | PHE | 277 | 20.676 | 45.674 | 106.952 | 1.00 | 20.12 | AAGL |
| ATOM | 2167 | N | LEU | 278 | 19.928 | 45.421 | 104.856 | 1.00 | 20.92 | AAGL |
| ATOM | 2168 | CA | LEU | 278 | 20.541 | 44.107 | 104.716 | 1.00 | 23.04 | AAGL |
| ATOM | 2169 | CB | LEU | 278 | 20.225 | 43.512 | 103.340 | 1.00 | 24.67 | AAGL |
| ATOM | 2170 | CG | LEU | 278 | 18.764 | 43.076 | 103.160 | 1.00 | 24.46 | AAGL |
| ATOM | 2171 | CD1 | LEU | 278 | 18.548 | 42.589 | 101.741 | 1.00 | 26.14 | AAGL |
| ATOM | 2172 | CD2 | LEU | 278 | 18.427 | 41.964 | 104.161 | 1.00 | 26.55 | AAGL |
| ATOM | 2173 | C | LEU | 278 | 22.040 | 44.144 | 104.947 | 1.00 | 23.23 | AAGL |
| ATOM | 2174 | O | LEU | 278 | 22.593 | 43.273 | 105.615 | 1.00 | 20.93 | AAGL |
| ATOM | 2175 | N | GLU | 279 | 22.707 | 45.155 | 104.404 | 1.00 | 24.22 | AAGL |
| ATOM | 2176 | CA | GLU | 279 | 24.141 | 45.244 | 104.601 | 1.00 | 25.09 | AAGL |
| ATOM | 2177 | CB | GLU | 279 | 24.735 | 46.309 | 103.682 | 1.00 | 26.59 | AAGL |
| ATOM | 2178 | CG | GLU | 279 | 24.418 | 46.045 | 102.213 | 1.00 | 32.07 | AAGL |
| ATOM | 2179 | CD | GLU | 279 | 25.419 | 46.691 | 101.274 | 1.00 | 37.00 | AAGL |
| ATOM | 2180 | OE1 | GLU | 279 | 25.859 | 47.815 | 101.576 | 1.00 | 39.68 | AAGL |
| ATOM | 2181 | OE2 | GLU | 279 | 25.756 | 46.078 | 100.235 | 1.00 | 40.09 | AAGL |
| ATOM | 2182 | C | GLU | 279 | 24.460 | 45.537 | 106.062 | 1.00 | 23.19 | AAGL |
| ATOM | 2183 | O | GLU | 279 | 25.409 | 44.984 | 106.614 | 1.00 | 23.97 | AAGL |
| ATOM | 2184 | N | LYS | 280 | 23.669 | 46.391 | 106.701 | 1.00 | 24.51 | AAGL |
| ATOM | 2185 | CA | LYS | 280 | 23.922 | 46.688 | 108.105 | 1.00 | 24.24 | AAGL |
| ATOM | 2186 | CB | LYS | 280 | 23.076 | 47.879 | 108.566 | 1.00 | 25.42 | AAGL |
| ATOM | 2187 | CG | LYS | 280 | 23.535 | 49.186 | 107.912 | 1.00 | 30.50 | AAGL |
| ATOM | 2188 | CD | LYS | 280 | 22.847 | 50.429 | 108.463 | 1.00 | 35.06 | AAGL |
| ATOM | 2189 | CE | LYS | 280 | 23.561 | 51.683 | 107.932 | 1.00 | 38.33 | AAGL |
| ATOM | 2190 | NZ | LYS | 280 | 23.003 | 52.962 | 108.460 | 1.00 | 39.58 | AAGL |
| ATOM | 2191 | C | LYS | 280 | 23.665 | 45.458 | 108.975 | 1.00 | 24.77 | AAGL |
| ATOM | 2192 | O | LYS | 280 | 24.382 | 45.219 | 109.949 | 1.00 | 21.68 | AAGL |
| ATOM | 2193 | N | LEU | 281 | 22.655 | 44.669 | 108.614 | 1.00 | 23.74 | AAGL |
| ATOM | 2194 | CA | LEU | 281 | 22.351 | 43.449 | 109.365 | 1.00 | 23.71 | AAGL |
| ATOM | 2195 | CB | LEU | 281 | 21.023 | 42.844 | 108.891 | 1.00 | 21.53 | AAGL |
| ATOM | 2196 | CG | LEU | 281 | 20.603 | 41.484 | 109.478 | 1.00 | 21.28 | AAGL |
| ATOM | 2197 | CD1 | LEU | 281 | 20.583 | 41.533 | 110.996 | 1.00 | 19.24 | AAGL |
| ATOM | 2198 | CD2 | LEU | 281 | 19.226 | 41.109 | 108.937 | 1.00 | 19.79 | AAGL |
| ATOM | 2199 | C | LEU | 281 | 23.482 | 42.429 | 109.172 | 1.00 | 22.36 | AAGL |

# Fig. 3 cont.

| ATOM | 2200 | O   | LEU | 281 | 23.940 | 41.803 | 110.125 | 1.00 | 24.16 | AAGL |
|------|------|-----|-----|-----|--------|--------|---------|------|-------|------|
| ATOM | 2201 | N   | ALA | 282 | 23.921 | 42.267 | 107.928 | 1.00 | 23.73 | AAGL |
| ATOM | 2202 | CA  | ALA | 282 | 24.998 | 41.339 | 107.611 | 1.00 | 23.94 | AAGL |
| ATOM | 2203 | CB  | ALA | 282 | 25.272 | 41.356 | 106.120 | 1.00 | 23.77 | AAGL |
| ATOM | 2204 | C   | ALA | 282 | 26.264 | 41.713 | 108.382 | 1.00 | 24.05 | AAGL |
| ATOM | 2205 | O   | ALA | 282 | 27.060 | 40.848 | 108.741 | 1.00 | 25.21 | AAGL |
| ATOM | 2206 | N   | ALA | 283 | 26.441 | 43.005 | 108.643 | 1.00 | 25.21 | AAGL |
| ATOM | 2207 | CA  | ALA | 283 | 27.614 | 43.477 | 109.372 | 1.00 | 25.75 | AAGL |
| ATOM | 2208 | CB  | ALA | 283 | 27.616 | 45.005 | 109.424 | 1.00 | 26.48 | AAGL |
| ATOM | 2209 | C   | ALA | 283 | 27.635 | 42.898 | 110.786 | 1.00 | 26.18 | AAGL |
| ATOM | 2210 | O   | ALA | 283 | 28.658 | 42.387 | 111.248 | 1.00 | 25.57 | AAGL |
| ATOM | 2211 | N   | VAL | 284 | 26.493 | 42.963 | 111.466 | 1.00 | 25.74 | AAGL |
| ATOM | 2212 | CA  | VAL | 284 | 26.383 | 42.438 | 112.824 | 1.00 | 25.11 | AAGL |
| ATOM | 2213 | CB  | VAL | 284 | 24.972 | 42.711 | 113.414 | 1.00 | 24.63 | AAGL |
| ATOM | 2214 | CG1 | VAL | 284 | 24.806 | 41.992 | 114.744 | 1.00 | 24.88 | AAGL |
| ATOM | 2215 | CG2 | VAL | 284 | 24.779 | 44.220 | 113.606 | 1.00 | 27.53 | AAGL |
| ATOM | 2216 | C   | VAL | 284 | 26.658 | 40.941 | 112.857 | 1.00 | 23.65 | AAGL |
| ATOM | 2217 | O   | VAL | 284 | 27.416 | 40.456 | 113.694 | 1.00 | 23.12 | AAGL |
| ATOM | 2218 | N   | VAL | 285 | 26.052 | 40.209 | 111.930 | 1.00 | 25.11 | AAGL |
| ATOM | 2219 | CA  | VAL | 285 | 26.236 | 38.769 | 111.881 | 1.00 | 23.69 | AAGL |
| ATOM | 2220 | CB  | VAL | 285 | 25.302 | 38.135 | 110.839 | 1.00 | 24.54 | AAGL |
| ATOM | 2221 | CG1 | VAL | 285 | 25.490 | 36.626 | 110.822 | 1.00 | 25.86 | AAGL |
| ATOM | 2222 | CG2 | VAL | 285 | 23.855 | 38.490 | 111.171 | 1.00 | 26.53 | AAGL |
| ATOM | 2223 | C   | VAL | 285 | 27.679 | 38.406 | 111.559 | 1.00 | 26.05 | AAGL |
| ATOM | 2224 | O   | VAL | 285 | 28.256 | 37.514 | 112.179 | 1.00 | 25.09 | AAGL |
| ATOM | 2225 | N   | GLU | 286 | 28.259 | 39.101 | 110.587 | 1.00 | 24.87 | AAGL |
| ATOM | 2226 | CA  | GLU | 286 | 29.639 | 38.847 | 110.201 | 1.00 | 26.91 | AAGL |
| ATOM | 2227 | CB  | GLU | 286 | 30.041 | 39.737 | 109.025 | 1.00 | 29.06 | AAGL |
| ATOM | 2228 | CG  | GLU | 286 | 31.518 | 39.586 | 108.629 | 1.00 | 32.60 | AAGL |
| ATOM | 2229 | CD  | GLU | 286 | 31.812 | 38.250 | 107.971 | 1.00 | 35.44 | AAGL |
| ATOM | 2230 | OE1 | GLU | 286 | 31.578 | 38.120 | 106.751 | 1.00 | 36.64 | AAGL |
| ATOM | 2231 | OE2 | GLU | 286 | 32.264 | 37.322 | 108.672 | 1.00 | 35.13 | AAGL |
| ATOM | 2232 | C   | GLU | 286 | 30.587 | 39.110 | 111.367 | 1.00 | 26.68 | AAGL |
| ATOM | 2233 | O   | GLU | 286 | 31.528 | 38.354 | 111.590 | 1.00 | 27.24 | AAGL |
| ATOM | 2234 | N   | ALA | 287 | 30.343 | 40.181 | 112.111 | 1.00 | 25.24 | AAGL |
| ATOM | 2235 | CA  | ALA | 287 | 31.211 | 40.522 | 113.230 | 1.00 | 27.43 | AAGL |
| ATOM | 2236 | CB  | ALA | 287 | 31.032 | 41.990 | 113.600 | 1.00 | 27.81 | AAGL |
| ATOM | 2237 | C   | ALA | 287 | 31.003 | 39.650 | 114.465 | 1.00 | 29.71 | AAGL |
| ATOM | 2238 | O   | ALA | 287 | 31.726 | 39.795 | 115.451 | 1.00 | 31.32 | AAGL |
| ATOM | 2239 | N   | THR | 288 | 30.024 | 38.749 | 114.415 | 1.00 | 28.83 | AAGL |
| ATOM | 2240 | CA  | THR | 288 | 29.744 | 37.871 | 115.549 | 1.00 | 29.55 | AAGL |
| ATOM | 2241 | CB  | THR | 288 | 28.242 | 37.499 | 115.618 | 1.00 | 28.36 | AAGL |
| ATOM | 2242 | OG1 | THR | 288 | 27.444 | 38.680 | 115.459 | 1.00 | 29.45 | AAGL |
| ATOM | 2243 | CG2 | THR | 288 | 27.921 | 36.854 | 116.962 | 1.00 | 31.36 | AAGL |
| ATOM | 2244 | C   | THR | 288 | 30.533 | 36.577 | 115.393 | 1.00 | 27.55 | AAGL |
| ATOM | 2245 | O   | THR | 288 | 30.708 | 36.094 | 114.280 | 1.00 | 27.21 | AAGL |
| ATOM | 2246 | N   | THR | 289 | 31.006 | 36.015 | 116.504 | 1.00 | 30.08 | AAGL |
| ATOM | 2247 | CA  | THR | 289 | 31.757 | 34.770 | 116.437 | 1.00 | 31.68 | AAGL |
| ATOM | 2248 | CB  | THR | 289 | 32.352 | 34.384 | 117.806 | 1.00 | 34.06 | AAGL |
| ATOM | 2249 | OG1 | THR | 289 | 33.186 | 35.449 | 118.291 | 1.00 | 35.86 | AAGL |
| ATOM | 2250 | CG2 | THR | 289 | 33.186 | 33.128 | 117.673 | 1.00 | 34.89 | AAGL |
| ATOM | 2251 | C   | THR | 289 | 30.817 | 33.659 | 115.964 | 1.00 | 33.04 | AAGL |
| ATOM | 2252 | O   | THR | 289 | 29.842 | 33.332 | 116.632 | 1.00 | 34.14 | AAGL |
| ATOM | 2253 | N   | ASP | 290 | 31.120 | 33.085 | 114.807 | 1.00 | 33.28 | AAGL |
| ATOM | 2254 | CA  | ASP | 290 | 30.298 | 32.030 | 114.211 | 1.00 | 32.82 | AAGL |
| ATOM | 2255 | CB  | ASP | 290 | 30.183 | 30.812 | 115.137 | 1.00 | 33.97 | AAGL |
| ATOM | 2256 | CG  | ASP | 290 | 31.397 | 29.900 | 115.054 | 1.00 | 38.26 | AAGL |
| ATOM | 2257 | OD1 | ASP | 290 | 32.093 | 29.921 | 114.006 | 1.00 | 38.79 | AAGL |
| ATOM | 2258 | OD2 | ASP | 290 | 31.651 | 29.152 | 116.024 | 1.00 | 38.34 | AAGL |
| ATOM | 2259 | C   | ASP | 290 | 28.903 | 32.495 | 113.793 | 1.00 | 30.86 | AAGL |
| ATOM | 2260 | O   | ASP | 290 | 27.909 | 31.781 | 113.979 | 1.00 | 31.04 | AAGL |
| ATOM | 2261 | N   | GLY | 291 | 28.841 | 33.705 | 113.246 | 1.00 | 30.92 | AAGL |
| ATOM | 2262 | CA  | GLY | 291 | 27.590 | 34.240 | 112.740 | 1.00 | 28.36 | AAGL |
| ATOM | 2263 | C   | GLY | 291 | 27.579 | 33.689 | 111.331 | 1.00 | 28.69 | AAGL |
| ATOM | 2264 | O   | GLY | 291 | 28.358 | 34.133 | 110.487 | 1.00 | 29.95 | AAGL |
| ATOM | 2265 | N   | LEU | 292 | 26.702 | 32.726 | 111.065 | 1.00 | 25.52 | AAGL |
| ATOM | 2266 | CA  | LEU | 292 | 26.662 | 32.072 | 109.767 | 1.00 | 25.89 | AAGL |

# Fig. 3 cont.

| ATOM | 2267 | CB | LEU | 292 | 26.184 | 30.632 | 109.940 | 1.00 | 25.46 | AAGL |
|------|------|-----|-----|-----|--------|--------|---------|------|-------|------|
| ATOM | 2268 | CG | LEU | 292 | 27.072 | 29.798 | 110.858 | 1.00 | 26.52 | AAGL |
| ATOM | 2269 | CD1 | LEU | 292 | 26.632 | 28.354 | 110.807 | 1.00 | 26.92 | AAGL |
| ATOM | 2270 | CD2 | LEU | 292 | 28.526 | 29.929 | 110.418 | 1.00 | 27.08 | AAGL |
| ATOM | 2271 | C | LEU | 292 | 25.908 | 32.700 | 108.613 | 1.00 | 25.35 | AAGL |
| ATOM | 2272 | O | LEU | 292 | 26.298 | 32.528 | 107.459 | 1.00 | 25.52 | AAGL |
| ATOM | 2273 | N | GLY | 293 | 24.824 | 33.413 | 108.887 | 1.00 | 25.75 | AAGL |
| ATOM | 2274 | CA | GLY | 293 | 24.118 | 33.990 | 107.769 | 1.00 | 22.89 | AAGL |
| ATOM | 2275 | C | GLY | 293 | 22.785 | 34.642 | 108.043 | 1.00 | 23.42 | AAGL |
| ATOM | 2276 | O | GLY | 293 | 22.366 | 34.828 | 109.187 | 1.00 | 21.61 | AAGL |
| ATOM | 2277 | N | VAL | 294 | 22.123 | 34.984 | 106.950 | 1.00 | 21.14 | AAGL |
| ATOM | 2278 | CA | VAL | 294 | 20.841 | 35.647 | 107.003 | 1.00 | 22.60 | AAGL |
| ATOM | 2279 | CB | VAL | 294 | 21.013 | 37.164 | 106.775 | 1.00 | 24.33 | AAGL |
| ATOM | 2280 | CG1 | VAL | 294 | 19.657 | 37.818 | 106.538 | 1.00 | 25.68 | AAGL |
| ATOM | 2281 | CG2 | VAL | 294 | 21.719 | 37.789 | 107.969 | 1.00 | 23.35 | AAGL |
| ATOM | 2282 | C | VAL | 294 | 19.926 | 35.094 | 105.932 | 1.00 | 23.50 | AAGL |
| ATOM | 2283 | O | VAL | 294 | 20.351 | 34.867 | 104.799 | 1.00 | 22.80 | AAGL |
| ATOM | 2284 | N | TYR | 295 | 18.668 | 34.871 | 106.293 | 1.00 | 21.62 | AAGL |
| ATOM | 2285 | CA | TYR | 295 | 17.684 | 34.387 | 105.338 | 1.00 | 20.32 | AAGL |
| ATOM | 2286 | CB | TYR | 295 | 17.105 | 33.035 | 105.761 | 1.00 | 20.96 | AAGL |
| ATOM | 2287 | CG | TYR | 295 | 18.040 | 31.862 | 105.606 | 1.00 | 21.66 | AAGL |
| ATOM | 2288 | CD1 | TYR | 295 | 19.124 | 31.692 | 106.461 | 1.00 | 20.77 | AAGL |
| ATOM | 2289 | CE1 | TYR | 295 | 19.974 | 30.584 | 106.337 | 1.00 | 22.52 | AAGL |
| ATOM | 2290 | CD2 | TYR | 295 | 17.820 | 30.904 | 104.617 | 1.00 | 21.20 | AAGL |
| ATOM | 2291 | CE2 | TYR | 295 | 18.658 | 29.798 | 104.481 | 1.00 | 22.01 | AAGL |
| ATOM | 2292 | CZ | TYR | 295 | 19.732 | 29.640 | 105.341 | 1.00 | 22.76 | AAGL |
| ATOM | 2293 | OH | TYR | 295 | 20.564 | 28.543 | 105.211 | 1.00 | 23.00 | AAGL |
| ATOM | 2294 | C | TYR | 295 | 16.554 | 35.399 | 105.295 | 1.00 | 21.79 | AAGL |
| ATOM | 2295 | O | TYR | 295 | 15.933 | 35.672 | 106.325 | 1.00 | 20.79 | AAGL |
| ATOM | 2296 | N | TYR | 296 | 16.296 | 35.966 | 104.118 | 1.00 | 20.08 | AAGL |
| ATOM | 2297 | CA | TYR | 296 | 15.212 | 36.927 | 103.975 | 1.00 | 19.64 | AAGL |
| ATOM | 2298 | CB | TYR | 296 | 15.328 | 37.704 | 102.666 | 1.00 | 20.69 | AAGL |
| ATOM | 2299 | CG | TYR | 296 | 14.503 | 38.972 | 102.656 | 1.00 | 19.70 | AAGL |
| ATOM | 2300 | CD1 | TYR | 296 | 15.005 | 40.152 | 103.194 | 1.00 | 21.48 | AAGL |
| ATOM | 2301 | CE1 | TYR | 296 | 14.236 | 41.310 | 103.232 | 1.00 | 21.48 | AAGL |
| ATOM | 2302 | CD2 | TYR | 296 | 13.203 | 38.980 | 102.147 | 1.00 | 19.37 | AAGL |
| ATOM | 2303 | CE2 | TYR | 296 | 12.423 | 40.138 | 102.182 | 1.00 | 21.23 | AAGL |
| ATOM | 2304 | CZ | TYR | 296 | 12.948 | 41.295 | 102.729 | 1.00 | 20.28 | AAGL |
| ATOM | 2305 | OH | TYR | 296 | 12.177 | 42.427 | 102.797 | 1.00 | 19.16 | AAGL |
| ATOM | 2306 | C | TYR | 296 | 13.947 | 36.090 | 103.939 | 1.00 | 20.23 | AAGL |
| ATOM | 2307 | O | TYR | 296 | 13.945 | 35.010 | 103.359 | 1.00 | 22.11 | AAGL |
| ATOM | 2308 | N | TRP | 297 | 12.868 | 36.578 | 104.538 | 1.00 | 17.43 | AAGL |
| ATOM | 2309 | CA | TRP | 297 | 11.641 | 35.795 | 104.553 | 1.00 | 17.69 | AAGL |
| ATOM | 2310 | CB | TRP | 297 | 10.942 | 35.894 | 105.920 | 1.00 | 19.08 | AAGL |
| ATOM | 2311 | CG | TRP | 297 | 9.854 | 34.864 | 106.075 | 1.00 | 19.30 | AAGL |
| ATOM | 2312 | CD2 | TRP | 297 | 8.440 | 35.098 | 106.104 | 1.00 | 19.62 | AAGL |
| ATOM | 2313 | CE2 | TRP | 297 | 7.808 | 33.837 | 106.201 | 1.00 | 20.98 | AAGL |
| ATOM | 2314 | CE3 | TRP | 297 | 7.644 | 36.250 | 106.057 | 1.00 | 21.65 | AAGL |
| ATOM | 2315 | CD1 | TRP | 297 | 10.018 | 33.511 | 106.155 | 1.00 | 21.34 | AAGL |
| ATOM | 2316 | NE1 | TRP | 297 | 8.793 | 32.885 | 106.231 | 1.00 | 21.42 | AAGL |
| ATOM | 2317 | CZ2 | TRP | 297 | 6.418 | 33.696 | 106.251 | 1.00 | 19.44 | AAGL |
| ATOM | 2318 | CZ3 | TRP | 297 | 6.257 | 36.109 | 106.106 | 1.00 | 24.11 | AAGL |
| ATOM | 2319 | CH2 | TRP | 297 | 5.661 | 34.836 | 106.201 | 1.00 | 22.67 | AAGL |
| ATOM | 2320 | C | TRP | 297 | 10.647 | 36.175 | 103.464 | 1.00 | 18.74 | AAGL |
| ATOM | 2321 | O | TRP | 297 | 10.158 | 37.305 | 103.428 | 1.00 | 17.76 | AAGL |
| ATOM | 2322 | N | GLU | 298 | 10.357 | 35.214 | 102.584 | 1.00 | 18.51 | AAGL |
| ATOM | 2323 | CA | GLU | 298 | 9.391 | 35.390 | 101.505 | 1.00 | 18.03 | AAGL |
| ATOM | 2324 | CB | GLU | 298 | 7.976 | 35.340 | 102.084 | 1.00 | 19.76 | AAGL |
| ATOM | 2325 | CG | GLU | 298 | 7.562 | 33.964 | 102.582 | 1.00 | 19.56 | AAGL |
| ATOM | 2326 | CD | GLU | 298 | 7.283 | 32.996 | 101.447 | 1.00 | 20.53 | AAGL |
| ATOM | 2327 | OE1 | GLU | 298 | 7.320 | 33.422 | 100.274 | 1.00 | 21.41 | AAGL |
| ATOM | 2328 | OE2 | GLU | 298 | 7.016 | 31.811 | 101.733 | 1.00 | 22.59 | AAGL |
| ATOM | 2329 | C | GLU | 298 | 9.553 | 36.664 | 100.668 | 1.00 | 20.54 | AAGL |
| ATOM | 2330 | O | GLU | 298 | 8.636 | 37.482 | 100.569 | 1.00 | 21.31 | AAGL |
| ATOM | 2331 | N | PRO | 299 | 10.715 | 36.832 | 100.025 | 1.00 | 21.16 | AAGL |
| ATOM | 2332 | CD | PRO | 299 | 11.893 | 35.949 | 100.046 | 1.00 | 20.70 | AAGL |
| ATOM | 2333 | CA | PRO | 299 | 10.964 | 38.022 | 99.203 | 1.00 | 21.46 | AAGL |

# Fig. 3 cont.

| ATOM | 2334 | CB | PRO | 299 | 12.455 | 37.913 | 98.897 | 1.00 | 22.49 | AAGL |
|------|------|-----|-----|-----|--------|--------|--------|------|-------|------|
| ATOM | 2335 | CG | PRO | 299 | 12.658 | 36.429 | 98.826 | 1.00 | 23.37 | AAGL |
| ATOM | 2336 | C | PRO | 299 | 10.133 | 38.131 | 97.924 | 1.00 | 21.34 | AAGL |
| ATOM | 2337 | O | PRO | 299 | 10.051 | 39.203 | 97.329 | 1.00 | 25.08 | AAGL |
| ATOM | 2338 | N | ALA | 300 | 9.515 | 37.031 | 97.507 | 1.00 | 21.73 | AAGL |
| ATOM | 2339 | CA | ALA | 300 | 8.751 | 37.021 | 96.264 | 1.00 | 23.94 | AAGL |
| ATOM | 2340 | CB | ALA | 300 | 9.418 | 36.071 | 95.272 | 1.00 | 23.80 | AAGL |
| ATOM | 2341 | C | ALA | 300 | 7.280 | 36.663 | 96.386 | 1.00 | 23.97 | AAGL |
| ATOM | 2342 | O | ALA | 300 | 6.663 | 36.277 | 95.394 | 1.00 | 24.57 | AAGL |
| ATOM | 2343 | N | TRP | 301 | 6.707 | 36.802 | 97.579 | 1.00 | 25.04 | AAGL |
| ATOM | 2344 | CA | TRP | 301 | 5.301 | 36.454 | 97.775 | 1.00 | 24.04 | AAGL |
| ATOM | 2345 | CB | TRP | 301 | 5.007 | 36.244 | 99.266 | 1.00 | 25.15 | AAGL |
| ATOM | 2346 | CG | TRP | 301 | 3.744 | 35.459 | 99.531 | 1.00 | 23.59 | AAGL |
| ATOM | 2347 | CD2 | TRP | 301 | 3.394 | 34.781 | 100.744 | 1.00 | 23.73 | AAGL |
| ATOM | 2348 | CE2 | TRP | 301 | 2.119 | 34.200 | 100.548 | 1.00 | 23.63 | AAGL |
| ATOM | 2349 | CE3 | TRP | 301 | 4.033 | 34.607 | 101.980 | 1.00 | 24.03 | AAGL |
| ATOM | 2350 | CD1 | TRP | 301 | 2.697 | 35.267 | 98.673 | 1.00 | 23.60 | AAGL |
| ATOM | 2351 | NE1 | TRP | 301 | 1.717 | 34.513 | 99.278 | 1.00 | 24.88 | AAGL |
| ATOM | 2352 | CZ2 | TRP | 301 | 1.470 | 33.458 | 101.544 | 1.00 | 22.63 | AAGL |
| ATOM | 2353 | CZ3 | TRP | 301 | 3.387 | 33.871 | 102.969 | 1.00 | 22.92 | AAGL |
| ATOM | 2354 | CH2 | TRP | 301 | 2.119 | 33.306 | 102.741 | 1.00 | 21.62 | AAGL |
| ATOM | 2355 | C | TRP | 301 | 4.322 | 37.485 | 97.213 | 1.00 | 25.72 | AAGL |
| ATOM | 2356 | O | TRP | 301 | 3.682 | 38.220 | 97.968 | 1.00 | 24.12 | AAGL |
| ATOM | 2357 | N | ILE | 302 | 4.192 | 37.532 | 95.889 | 1.00 | 26.27 | AAGL |
| ATOM | 2358 | CA | ILE | 302 | 3.273 | 38.475 | 95.256 | 1.00 | 26.33 | AAGL |
| ATOM | 2359 | CB | ILE | 302 | 3.257 | 38.317 | 93.722 | 1.00 | 28.94 | AAGL |
| ATOM | 2360 | CG2 | ILE | 302 | 2.804 | 39.615 | 93.081 | 1.00 | 30.12 | AAGL |
| ATOM | 2361 | CG1 | ILE | 302 | 4.653 | 37.963 | 93.215 | 1.00 | 32.05 | AAGL |
| ATOM | 2362 | CD1 | ILE | 302 | 5.671 | 39.038 | 93.462 | 1.00 | 33.22 | AAGL |
| ATOM | 2363 | C | ILE | 302 | 1.872 | 38.180 | 95.770 | 1.00 | 24.91 | AAGL |
| ATOM | 2364 | O | ILE | 302 | 1.467 | 37.017 | 95.840 | 1.00 | 26.39 | AAGL |
| ATOM | 2365 | N | GLY | 303 | 1.134 | 39.223 | 96.133 | 1.00 | 25.25 | AAGL |
| ATOM | 2366 | CA | GLY | 303 | -0.210 | 39.018 | 96.646 | 1.00 | 27.25 | AAGL |
| ATOM | 2367 | C | GLY | 303 | -0.298 | 39.086 | 98.159 | 1.00 | 26.83 | AAGL |
| ATOM | 2368 | O | GLY | 303 | -1.394 | 39.110 | 98.728 | 1.00 | 27.53 | AAGL |
| ATOM | 2369 | N | ASN | 304 | 0.861 | 39.090 | 98.812 | 1.00 | 25.82 | AAGL |
| ATOM | 2370 | CA | ASN | 304 | 0.958 | 39.182 | 100.267 | 1.00 | 23.80 | AAGL |
| ATOM | 2371 | CB | ASN | 304 | 1.113 | 37.783 | 100.887 | 1.00 | 22.97 | AAGL |
| ATOM | 2372 | CG | ASN | 304 | 1.131 | 37.811 | 102.413 | 1.00 | 23.62 | AAGL |
| ATOM | 2373 | OD1 | ASN | 304 | 0.494 | 38.663 | 103.038 | 1.00 | 25.26 | AAGL |
| ATOM | 2374 | ND2 | ASN | 304 | 1.841 | 36.864 | 103.017 | 1.00 | 20.66 | AAGL |
| ATOM | 2375 | C | ASN | 304 | 2.200 | 40.031 | 100.539 | 1.00 | 22.75 | AAGL |
| ATOM | 2376 | O | ASN | 304 | 3.030 | 39.704 | 101.382 | 1.00 | 21.47 | AAGL |
| ATOM | 2377 | N | ALA | 305 | 2.306 | 41.139 | 99.812 | 1.00 | 23.77 | AAGL |
| ATOM | 2378 | CA | ALA | 305 | 3.454 | 42.028 | 99.926 | 1.00 | 23.13 | AAGL |
| ATOM | 2379 | CB | ALA | 305 | 3.281 | 43.211 | 98.980 | 1.00 | 25.11 | AAGL |
| ATOM | 2380 | C | ALA | 305 | 3.770 | 42.520 | 101.335 | 1.00 | 22.70 | AAGL |
| ATOM | 2381 | O | ALA | 305 | 4.928 | 42.784 | 101.650 | 1.00 | 23.39 | AAGL |
| ATOM | 2382 | N | GLY | 306 | 2.753 | 42.632 | 102.182 | 1.00 | 23.04 | AAGL |
| ATOM | 2383 | CA | GLY | 306 | 2.970 | 43.093 | 103.543 | 1.00 | 21.61 | AAGL |
| ATOM | 2384 | C | GLY | 306 | 3.592 | 42.023 | 104.421 | 1.00 | 20.83 | AAGL |
| ATOM | 2385 | O | GLY | 306 | 4.185 | 42.323 | 105.461 | 1.00 | 20.31 | AAGL |
| ATOM | 2386 | N | LEU | 307 | 3.445 | 40.771 | 103.997 | 1.00 | 20.88 | AAGL |
| ATOM | 2387 | CA | LEU | 307 | 3.980 | 39.615 | 104.710 | 1.00 | 19.63 | AAGL |
| ATOM | 2388 | CB | LEU | 307 | 5.511 | 39.575 | 104.599 | 1.00 | 19.26 | AAGL |
| ATOM | 2389 | CG | LEU | 307 | 6.089 | 39.333 | 103.198 | 1.00 | 17.07 | AAGL |
| ATOM | 2390 | CD1 | LEU | 307 | 7.602 | 39.293 | 103.292 | 1.00 | 21.74 | AAGL |
| ATOM | 2391 | CD2 | LEU | 307 | 5.568 | 38.012 | 102.625 | 1.00 | 18.50 | AAGL |
| ATOM | 2392 | C | LEU | 307 | 3.580 | 39.543 | 106.178 | 1.00 | 20.69 | AAGL |
| ATOM | 2393 | O | LEU | 307 | 4.377 | 39.131 | 107.018 | 1.00 | 20.75 | AAGL |
| ATOM | 2394 | N | GLY | 308 | 2.352 | 39.955 | 106.484 | 1.00 | 19.76 | AAGL |
| ATOM | 2395 | CA | GLY | 308 | 1.870 | 39.898 | 107.854 | 1.00 | 22.38 | AAGL |
| ATOM | 2396 | C | GLY | 308 | 2.188 | 41.068 | 108.769 | 1.00 | 23.64 | AAGL |
| ATOM | 2397 | O | GLY | 308 | 1.785 | 41.072 | 109.938 | 1.00 | 23.65 | AAGL |
| ATOM | 2398 | N | SER | 309 | 2.907 | 42.060 | 108.252 | 1.00 | 23.88 | AAGL |
| ATOM | 2399 | CA | SER | 309 | 3.275 | 43.227 | 109.045 | 1.00 | 22.50 | AAGL |
| ATOM | 2400 | CB | SER | 309 | 4.693 | 43.684 | 108.695 | 1.00 | 22.00 | AAGL |

# Fig. 3 cont.

| ATOM | 2401 | OG  | SER | 309 | 4.719  | 44.264 | 107.407 | 1.00 | 20.09 | AAGL |
|------|------|-----|-----|-----|--------|--------|---------|------|-------|------|
| ATOM | 2402 | C   | SER | 309 | 2.312  | 44.385 | 108.790 | 1.00 | 23.02 | AAGL |
| ATOM | 2403 | O   | SER | 309 | 1.388  | 44.271 | 107.983 | 1.00 | 23.42 | AAGL |
| ATOM | 2404 | N   | SER | 310 | 2.539  | 45.494 | 109.486 | 1.00 | 20.79 | AAGL |
| ATOM | 2405 | CA  | SER | 310 | 1.707  | 46.684 | 109.316 | 1.00 | 23.22 | AAGL |
| ATOM | 2406 | CB  | SER | 310 | 1.715  | 47.535 | 110.592 | 1.00 | 22.59 | AAGL |
| ATOM | 2407 | OG  | SER | 310 | 3.022  | 48.003 | 110.903 | 1.00 | 24.03 | AAGL |
| ATOM | 2408 | C   | SER | 310 | 2.234  | 47.512 | 108.138 | 1.00 | 23.44 | AAGL |
| ATOM | 2409 | O   | SER | 310 | 1.658  | 48.545 | 107.773 | 1.00 | 23.68 | AAGL |
| ATOM | 2410 | N   | CYS | 311 | 3.340  | 47.069 | 107.548 | 1.00 | 21.68 | AAGL |
| ATOM | 2411 | CA  | CYS | 311 | 3.892  | 47.788 | 106.413 | 1.00 | 23.63 | AAGL |
| ATOM | 2412 | C   | CYS | 311 | 3.210  | 47.381 | 105.123 | 1.00 | 24.17 | AAGL |
| ATOM | 2413 | O   | CYS | 311 | 2.591  | 46.321 | 105.044 | 1.00 | 26.98 | AAGL |
| ATOM | 2414 | CB  | CYS | 311 | 5.387  | 47.545 | 106.289 | 1.00 | 25.30 | AAGL |
| ATOM | 2415 | SG  | CYS | 311 | 6.407  | 48.425 | 107.501 | 1.00 | 27.01 | AAGL |
| ATOM | 2416 | N   | ALA | 312 | 3.343  | 48.219 | 104.104 | 1.00 | 23.57 | AAGL |
| ATOM | 2417 | CA  | ALA | 312 | 2.707  | 47.954 | 102.821 | 1.00 | 25.20 | AAGL |
| ATOM | 2418 | CB  | ALA | 312 | 2.516  | 49.266 | 102.053 | 1.00 | 25.76 | AAGL |
| ATOM | 2419 | C   | ALA | 312 | 3.400  | 46.950 | 101.919 | 1.00 | 25.50 | AAGL |
| ATOM | 2420 | O   | ALA | 312 | 2.741  | 46.128 | 101.288 | 1.00 | 24.61 | AAGL |
| ATOM | 2421 | N   | ASP | 313 | 4.726  | 47.003 | 101.858 | 1.00 | 25.50 | AAGL |
| ATOM | 2422 | CA  | ASP | 313 | 5.444  | 46.122 | 100.949 | 1.00 | 25.55 | AAGL |
| ATOM | 2423 | CB  | ASP | 313 | 5.560  | 46.827 | 99.596  | 1.00 | 28.83 | AAGL |
| ATOM | 2424 | CG  | ASP | 313 | 5.870  | 45.886 | 98.471  | 1.00 | 31.63 | AAGL |
| ATOM | 2425 | OD1 | ASP | 313 | 6.652  | 44.940 | 98.680  | 1.00 | 29.42 | AAGL |
| ATOM | 2426 | OD2 | ASP | 313 | 5.337  | 46.107 | 97.358  | 1.00 | 37.09 | AAGL |
| ATOM | 2427 | C   | ASP | 313 | 6.836  | 45.752 | 101.440 | 1.00 | 25.26 | AAGL |
| ATOM | 2428 | O   | ASP | 313 | 7.698  | 46.620 | 101.575 | 1.00 | 25.34 | AAGL |
| ATOM | 2429 | N   | ASN | 314 | 7.049  | 44.460 | 101.685 | 1.00 | 22.30 | AAGL |
| ATOM | 2430 | CA  | ASN | 314 | 8.335  | 43.956 | 102.157 | 1.00 | 21.78 | AAGL |
| ATOM | 2431 | CB  | ASN | 314 | 8.156  | 43.167 | 103.458 | 1.00 | 23.69 | AAGL |
| ATOM | 2432 | CG  | ASN | 314 | 7.832  | 44.056 | 104.640 | 1.00 | 25.29 | AAGL |
| ATOM | 2433 | OD1 | ASN | 314 | 8.520  | 45.039 | 104.883 | 1.00 | 28.43 | AAGL |
| ATOM | 2434 | ND2 | ASN | 314 | 6.787  | 43.710 | 105.382 | 1.00 | 24.92 | AAGL |
| ATOM | 2435 | C   | ASN | 314 | 8.999  | 43.053 | 101.127 | 1.00 | 22.83 | AAGL |
| ATOM | 2436 | O   | ASN | 314 | 10.043 | 42.469 | 101.393 | 1.00 | 21.72 | AAGL |
| ATOM | 2437 | N   | LEU | 315 | 8.388  | 42.942 | 99.955  | 1.00 | 22.78 | AAGL |
| ATOM | 2438 | CA  | LEU | 315 | 8.919  | 42.086 | 98.907  | 1.00 | 22.99 | AAGL |
| ATOM | 2439 | CB  | LEU | 315 | 7.879  | 41.913 | 97.796  | 1.00 | 22.49 | AAGL |
| ATOM | 2440 | CG  | LEU | 315 | 6.491  | 41.421 | 98.219  | 1.00 | 22.62 | AAGL |
| ATOM | 2441 | CD1 | LEU | 315 | 5.599  | 41.214 | 96.991  | 1.00 | 25.48 | AAGL |
| ATOM | 2442 | CD2 | LEU | 315 | 6.638  | 40.117 | 98.978  | 1.00 | 23.90 | AAGL |
| ATOM | 2443 | C   | LEU | 315 | 10.219 | 42.604 | 98.310  | 1.00 | 24.65 | AAGL |
| ATOM | 2444 | O   | LEU | 315 | 10.608 | 43.756 | 98.523  | 1.00 | 24.23 | AAGL |
| ATOM | 2445 | N   | MET | 316 | 10.898 | 41.728 | 97.576  | 1.00 | 25.62 | AAGL |
| ATOM | 2446 | CA  | MET | 316 | 12.135 | 42.088 | 96.901  | 1.00 | 28.28 | AAGL |
| ATOM | 2447 | CB  | MET | 316 | 13.280 | 41.159 | 97.321  | 1.00 | 26.81 | AAGL |
| ATOM | 2448 | CG  | MET | 316 | 13.718 | 41.299 | 98.777  | 1.00 | 27.89 | AAGL |
| ATOM | 2449 | SD  | MET | 316 | 15.182 | 40.302 | 99.187  | 1.00 | 29.46 | AAGL |
| ATOM | 2450 | CE  | MET | 316 | 16.470 | 41.485 | 98.890  | 1.00 | 29.41 | AAGL |
| ATOM | 2451 | C   | MET | 316 | 11.889 | 41.977 | 95.393  | 1.00 | 29.33 | AAGL |
| ATOM | 2452 | O   | MET | 316 | 12.824 | 41.939 | 94.599  | 1.00 | 29.21 | AAGL |
| ATOM | 2453 | N   | VAL | 317 | 10.616 | 41.910 | 95.015  | 1.00 | 30.78 | AAGL |
| ATOM | 2454 | CA  | VAL | 317 | 10.217 | 41.820 | 93.614  | 1.00 | 32.20 | AAGL |
| ATOM | 2455 | CB  | VAL | 317 | 9.681  | 40.416 | 93.263  | 1.00 | 31.88 | AAGL |
| ATOM | 2456 | CG1 | VAL | 317 | 10.763 | 39.374 | 93.477  | 1.00 | 33.90 | AAGL |
| ATOM | 2457 | CG2 | VAL | 317 | 8.479  | 40.100 | 94.128  | 1.00 | 36.43 | AAGL |
| ATOM | 2458 | C   | VAL | 317 | 9.113  | 42.836 | 93.346  | 1.00 | 33.46 | AAGL |
| ATOM | 2459 | O   | VAL | 317 | 8.342  | 43.169 | 94.246  | 1.00 | 30.98 | AAGL |
| ATOM | 2460 | N   | ASP | 318 | 9.041  | 43.333 | 92.113  | 1.00 | 33.99 | AAGL |
| ATOM | 2461 | CA  | ASP | 318 | 8.015  | 44.309 | 91.760  | 1.00 | 38.16 | AAGL |
| ATOM | 2462 | CB  | ASP | 318 | 8.405  | 45.073 | 90.493  | 1.00 | 39.54 | AAGL |
| ATOM | 2463 | CG  | ASP | 318 | 7.502  | 46.252 | 90.240  | 1.00 | 38.96 | AAGL |
| ATOM | 2464 | OD1 | ASP | 318 | 6.267  | 46.066 | 90.216  | 1.00 | 40.93 | AAGL |
| ATOM | 2465 | OD2 | ASP | 318 | 8.022  | 47.370 | 90.058  | 1.00 | 42.03 | AAGL |
| ATOM | 2466 | C   | ASP | 318 | 6.671  | 43.621 | 91.547  | 1.00 | 41.03 | AAGL |
| ATOM | 2467 | O   | ASP | 318 | 6.512  | 42.800 | 90.642  | 1.00 | 41.02 | AAGL |

# Fig. 3 cont.

| ATOM | 2468 | N   | TYR | 319 | 5.695  | 43.985 | 92.373 | 1.00 | 43.91 | AAGL |
|------|------|-----|-----|-----|--------|--------|--------|------|-------|------|
| ATOM | 2469 | CA  | TYR | 319 | 4.370  | 43.388 | 92.312 | 1.00 | 46.99 | AAGL |
| ATOM | 2470 | CB  | TYR | 319 | 3.555  | 43.811 | 93.548 | 1.00 | 48.59 | AAGL |
| ATOM | 2471 | CG  | TYR | 319 | 3.003  | 45.224 | 93.516 | 1.00 | 48.66 | AAGL |
| ATOM | 2472 | CD1 | TYR | 319 | 1.702  | 45.475 | 93.080 | 1.00 | 49.01 | AAGL |
| ATOM | 2473 | CE1 | TYR | 319 | 1.180  | 46.778 | 93.066 | 1.00 | 49.49 | AAGL |
| ATOM | 2474 | CD2 | TYR | 319 | 3.772  | 46.305 | 93.937 | 1.00 | 49.12 | AAGL |
| ATOM | 2475 | CE2 | TYR | 319 | 3.264  | 47.610 | 93.929 | 1.00 | 49.13 | AAGL |
| ATOM | 2476 | CZ  | TYR | 319 | 1.967  | 47.836 | 93.493 | 1.00 | 49.15 | AAGL |
| ATOM | 2477 | OH  | TYR | 319 | 1.457  | 49.115 | 93.495 | 1.00 | 48.83 | AAGL |
| ATOM | 2478 | C   | TYR | 319 | 3.602  | 43.705 | 91.034 | 1.00 | 49.01 | AAGL |
| ATOM | 2479 | O   | TYR | 319 | 2.479  | 43.221 | 90.840 | 1.00 | 51.46 | AAGL |
| ATOM | 2480 | N   | THR | 320 | 4.178  | 44.522 | 90.158 | 1.00 | 48.98 | AAGL |
| ATOM | 2481 | CA  | THR | 320 | 3.491  | 44.827 | 88.909 | 1.00 | 48.98 | AAGL |
| ATOM | 2482 | CB  | THR | 320 | 3.383  | 46.349 | 88.642 | 1.00 | 48.87 | AAGL |
| ATOM | 2483 | OG1 | THR | 320 | 4.681  | 46.899 | 88.371 | 1.00 | 48.24 | AAGL |
| ATOM | 2484 | CG2 | THR | 320 | 2.770  | 47.054 | 89.829 | 1.00 | 48.99 | AAGL |
| ATOM | 2485 | C   | THR | 320 | 4.206  | 44.184 | 87.730 | 1.00 | 49.75 | AAGL |
| ATOM | 2486 | O   | THR | 320 | 3.572  | 43.536 | 86.896 | 1.00 | 50.61 | AAGL |
| ATOM | 2487 | N   | THR | 321 | 5.524  | 44.349 | 87.671 | 1.00 | 49.77 | AAGL |
| ATOM | 2488 | CA  | THR | 321 | 6.316  | 43.798 | 86.575 | 1.00 | 50.22 | AAGL |
| ATOM | 2489 | CB  | THR | 321 | 7.561  | 44.673 | 86.297 | 1.00 | 50.80 | AAGL |
| ATOM | 2490 | OG1 | THR | 321 | 8.505  | 44.522 | 87.368 | 1.00 | 51.66 | AAGL |
| ATOM | 2491 | CG2 | THR | 321 | 7.168  | 46.144 | 86.193 | 1.00 | 51.57 | AAGL |
| ATOM | 2492 | C   | THR | 321 | 6.805  | 42.371 | 86.807 | 1.00 | 50.00 | AAGL |
| ATOM | 2493 | O   | THR | 321 | 7.360  | 41.743 | 85.905 | 1.00 | 50.77 | AAGL |
| ATOM | 2494 | N   | ASP | 322 | 6.617  | 41.859 | 88.016 | 1.00 | 49.25 | AAGL |
| ATOM | 2495 | CA  | ASP | 322 | 7.082  | 40.515 | 88.345 | 1.00 | 47.20 | AAGL |
| ATOM | 2496 | CB  | ASP | 322 | 6.534  | 39.471 | 87.354 | 1.00 | 50.64 | AAGL |
| ATOM | 2497 | CG  | ASP | 322 | 5.010  | 39.462 | 87.262 | 1.00 | 52.01 | AAGL |
| ATOM | 2498 | OD1 | ASP | 322 | 4.313  | 39.445 | 88.309 | 1.00 | 52.82 | AAGL |
| ATOM | 2499 | OD2 | ASP | 322 | 4.502  | 39.442 | 86.113 | 1.00 | 55.12 | AAGL |
| ATOM | 2500 | C   | ASP | 322 | 8.616  | 40.486 | 88.288 | 1.00 | 44.47 | AAGL |
| ATOM | 2501 | O   | ASP | 322 | 9.231  | 39.416 | 88.385 | 1.00 | 44.83 | AAGL |
| ATOM | 2502 | N   | GLU | 323 | 9.236  | 41.652 | 88.124 | 1.00 | 41.39 | AAGL |
| ATOM | 2503 | CA  | GLU | 323 | 10.696 | 41.745 | 88.049 | 1.00 | 39.30 | AAGL |
| ATOM | 2504 | CB  | GLU | 323 | 11.093 | 42.894 | 87.127 | 1.00 | 41.31 | AAGL |
| ATOM | 2505 | CG  | GLU | 323 | 12.586 | 43.108 | 86.977 | 1.00 | 44.75 | AAGL |
| ATOM | 2506 | CD  | GLU | 323 | 12.911 | 44.040 | 85.812 | 1.00 | 47.16 | AAGL |
| ATOM | 2507 | OE1 | GLU | 323 | 14.099 | 44.371 | 85.612 | 1.00 | 47.71 | AAGL |
| ATOM | 2508 | OE2 | GLU | 323 | 11.971 | 44.438 | 85.091 | 1.00 | 47.99 | AAGL |
| ATOM | 2509 | C   | GLU | 323 | 11.346 | 41.939 | 89.420 | 1.00 | 36.82 | AAGL |
| ATOM | 2510 | O   | GLU | 323 | 10.898 | 42.761 | 90.220 | 1.00 | 35.46 | AAGL |
| ATOM | 2511 | N   | VAL | 324 | 12.410 | 41.182 | 89.675 | 1.00 | 35.31 | AAGL |
| ATOM | 2512 | CA  | VAL | 324 | 13.120 | 41.257 | 90.948 | 1.00 | 32.93 | AAGL |
| ATOM | 2513 | CB  | VAL | 324 | 14.154 | 40.103 | 91.099 | 1.00 | 33.31 | AAGL |
| ATOM | 2514 | CG1 | VAL | 324 | 13.487 | 38.770 | 90.827 | 1.00 | 32.75 | AAGL |
| ATOM | 2515 | CG2 | VAL | 324 | 15.341 | 40.316 | 90.153 | 1.00 | 32.38 | AAGL |
| ATOM | 2516 | C   | VAL | 324 | 13.864 | 42.573 | 91.090 | 1.00 | 33.56 | AAGL |
| ATOM | 2517 | O   | VAL | 324 | 14.329 | 43.153 | 90.093 | 1.00 | 33.29 | AAGL |
| ATOM | 2518 | N   | TYR | 325 | 13.974 | 43.045 | 92.328 | 1.00 | 30.85 | AAGL |
| ATOM | 2519 | CA  | TYR | 325 | 14.683 | 44.282 | 92.608 | 1.00 | 31.59 | AAGL |
| ATOM | 2520 | CB  | TYR | 325 | 14.228 | 44.910 | 93.929 | 1.00 | 30.31 | AAGL |
| ATOM | 2521 | CG  | TYR | 325 | 12.794 | 45.387 | 93.972 | 1.00 | 31.58 | AAGL |
| ATOM | 2522 | CD1 | TYR | 325 | 12.225 | 46.079 | 92.901 | 1.00 | 31.55 | AAGL |
| ATOM | 2523 | CE1 | TYR | 325 | 10.908 | 46.548 | 92.970 | 1.00 | 33.68 | AAGL |
| ATOM | 2524 | CD2 | TYR | 325 | 12.015 | 45.177 | 95.112 | 1.00 | 30.63 | AAGL |
| ATOM | 2525 | CE2 | TYR | 325 | 10.714 | 45.639 | 95.192 | 1.00 | 30.81 | AAGL |
| ATOM | 2526 | CZ  | TYR | 325 | 10.164 | 46.323 | 94.127 | 1.00 | 33.10 | AAGL |
| ATOM | 2527 | OH  | TYR | 325 | 8.878  | 46.780 | 94.231 | 1.00 | 32.89 | AAGL |
| ATOM | 2528 | C   | TYR | 325 | 16.169 | 44.003 | 92.714 | 1.00 | 31.02 | AAGL |
| ATOM | 2529 | O   | TYR | 325 | 16.602 | 42.859 | 92.908 | 1.00 | 28.70 | AAGL |
| ATOM | 2530 | N   | GLU | 326 | 16.946 | 45.070 | 92.599 | 1.00 | 31.64 | AAGL |
| ATOM | 2531 | CA  | GLU | 326 | 18.398 | 45.010 | 92.684 | 1.00 | 31.11 | AAGL |
| ATOM | 2532 | CB  | GLU | 326 | 18.949 | 46.406 | 92.388 | 1.00 | 34.73 | AAGL |
| ATOM | 2533 | CG  | GLU | 326 | 20.432 | 46.588 | 92.571 | 1.00 | 39.05 | AAGL |
| ATOM | 2534 | CD  | GLU | 326 | 20.851 | 47.994 | 92.209 | 1.00 | 41.46 | AAGL |

# Fig. 3 cont.

| ATOM | 2535 | OE1 | GLU | 326 | 20.682 | 48.359 | 91.021 | 1.00 | 42.66 | AAGL |
|------|------|-----|-----|-----|--------|--------|--------|------|-------|------|
| ATOM | 2536 | OE2 | GLU | 326 | 21.334 | 48.731 | 93.106 | 1.00 | 40.82 | AAGL |
| ATOM | 2537 | C | GLU | 326 | 18.848 | 44.538 | 94.065 | 1.00 | 29.10 | AAGL |
| ATOM | 2538 | O | GLU | 326 | 19.996 | 44.136 | 94.253 | 1.00 | 27.19 | AAGL |
| ATOM | 2539 | N | SER | 327 | 17.939 | 44.581 | 95.035 | 1.00 | 27.41 | AAGL |
| ATOM | 2540 | CA | SER | 327 | 18.265 | 44.147 | 96.387 | 1.00 | 25.31 | AAGL |
| ATOM | 2541 | CB | SER | 327 | 17.127 | 44.519 | 97.347 | 1.00 | 23.59 | AAGL |
| ATOM | 2542 | OG | SER | 327 | 15.870 | 44.218 | 96.776 | 1.00 | 25.25 | AAGL |
| ATOM | 2543 | C | SER | 327 | 18.574 | 42.650 | 96.458 | 1.00 | 24.17 | AAGL |
| ATOM | 2544 | O | SER | 327 | 19.243 | 42.195 | 97.383 | 1.00 | 25.88 | AAGL |
| ATOM | 2545 | N | ILE | 328 | 18.107 | 41.880 | 95.479 | 1.00 | 27.45 | AAGL |
| ATOM | 2546 | CA | ILE | 328 | 18.395 | 40.446 | 95.466 | 1.00 | 28.86 | AAGL |
| ATOM | 2547 | CB | ILE | 328 | 17.692 | 39.728 | 94.295 | 1.00 | 31.12 | AAGL |
| ATOM | 2548 | CG2 | ILE | 328 | 18.120 | 38.277 | 94.250 | 1.00 | 35.58 | AAGL |
| ATOM | 2549 | CG1 | ILE | 328 | 16.175 | 39.823 | 94.448 | 1.00 | 33.48 | AAGL |
| ATOM | 2550 | CD1 | ILE | 328 | 15.647 | 39.194 | 95.727 | 1.00 | 36.80 | AAGL |
| ATOM | 2551 | C | ILE | 328 | 19.904 | 40.248 | 95.317 | 1.00 | 29.16 | AAGL |
| ATOM | 2552 | O | ILE | 328 | 20.486 | 39.324 | 95.897 | 1.00 | 27.50 | AAGL |
| ATOM | 2553 | N | GLU | 329 | 20.536 | 41.124 | 94.538 | 1.00 | 30.01 | AAGL |
| ATOM | 2554 | CA | GLU | 329 | 21.978 | 41.045 | 94.328 | 1.00 | 30.96 | AAGL |
| ATOM | 2555 | CB | GLU | 329 | 22.435 | 42.017 | 93.229 | 1.00 | 33.99 | AAGL |
| ATOM | 2556 | CG | GLU | 329 | 21.773 | 41.813 | 91.866 | 1.00 | 37.96 | AAGL |
| ATOM | 2557 | CD | GLU | 329 | 22.520 | 42.542 | 90.746 | 1.00 | 42.17 | AAGL |
| ATOM | 2558 | OE1 | GLU | 329 | 22.731 | 43.773 | 90.863 | 1.00 | 42.73 | AAGL |
| ATOM | 2559 | OE2 | GLU | 329 | 22.898 | 41.883 | 89.746 | 1.00 | 42.99 | AAGL |
| ATOM | 2560 | C | GLU | 329 | 22.682 | 41.386 | 95.627 | 1.00 | 29.64 | AAGL |
| ATOM | 2561 | O | GLU | 329 | 23.693 | 40.771 | 95.988 | 1.00 | 29.09 | AAGL |
| ATOM | 2562 | N | THR | 330 | 22.142 | 42.368 | 96.340 | 1.00 | 28.03 | AAGL |
| ATOM | 2563 | CA | THR | 330 | 22.720 | 42.776 | 97.611 | 1.00 | 26.58 | AAGL |
| ATOM | 2564 | CB | THR | 330 | 21.958 | 43.986 | 98.200 | 1.00 | 27.90 | AAGL |
| ATOM | 2565 | OG1 | THR | 330 | 22.099 | 45.110 | 97.323 | 1.00 | 26.78 | AAGL |
| ATOM | 2566 | CG2 | THR | 330 | 22.495 | 44.345 | 99.574 | 1.00 | 27.91 | AAGL |
| ATOM | 2567 | C | THR | 330 | 22.671 | 41.608 | 98.606 | 1.00 | 26.92 | AAGL |
| ATOM | 2568 | O | THR | 330 | 23.654 | 41.325 | 99.301 | 1.00 | 25.31 | AAGL |
| ATOM | 2569 | N | LEU | 331 | 21.529 | 40.930 | 98.667 | 1.00 | 25.72 | AAGL |
| ATOM | 2570 | CA | LEU | 331 | 21.368 | 39.791 | 99.571 | 1.00 | 24.97 | AAGL |
| ATOM | 2571 | CB | LEU | 331 | 19.923 | 39.282 | 99.532 | 1.00 | 24.19 | AAGL |
| ATOM | 2572 | CG | LEU | 331 | 19.567 | 37.968 | 100.247 | 1.00 | 23.31 | AAGL |
| ATOM | 2573 | CD1 | LEU | 331 | 19.873 | 38.051 | 101.736 | 1.00 | 25.91 | AAGL |
| ATOM | 2574 | CD2 | LEU | 331 | 18.082 | 37.674 | 100.034 | 1.00 | 23.20 | AAGL |
| ATOM | 2575 | C | LEU | 331 | 22.319 | 38.674 | 99.158 | 1.00 | 25.90 | AAGL |
| ATOM | 2576 | O | LEU | 331 | 22.971 | 38.054 | 100.001 | 1.00 | 25.54 | AAGL |
| ATOM | 2577 | N | GLY | 332 | 22.390 | 38.427 | 97.853 | 1.00 | 26.10 | AAGL |
| ATOM | 2578 | CA | GLY | 332 | 23.262 | 37.386 | 97.337 | 1.00 | 28.89 | AAGL |
| ATOM | 2579 | C | GLY | 332 | 24.738 | 37.631 | 97.594 | 1.00 | 31.12 | AAGL |
| ATOM | 2580 | O | GLY | 332 | 25.526 | 36.682 | 97.614 | 1.00 | 30.65 | AAGL |
| ATOM | 2581 | N | GLU | 333 | 25.120 | 38.890 | 97.805 | 1.00 | 31.60 | AAGL |
| ATOM | 2582 | CA | GLU | 333 | 26.524 | 39.229 | 98.044 | 1.00 | 33.74 | AAGL |
| ATOM | 2583 | CB | GLU | 333 | 26.949 | 40.400 | 97.148 | 1.00 | 34.97 | AAGL |
| ATOM | 2584 | CG | GLU | 333 | 26.639 | 40.205 | 95.673 | 1.00 | 37.79 | AAGL |
| ATOM | 2585 | CD | GLU | 333 | 26.846 | 41.471 | 94.846 | 1.00 | 41.19 | AAGL |
| ATOM | 2586 | OE1 | GLU | 333 | 26.164 | 41.621 | 93.807 | 1.00 | 40.67 | AAGL |
| ATOM | 2587 | OE2 | GLU | 333 | 27.694 | 42.309 | 95.225 | 1.00 | 44.05 | AAGL |
| ATOM | 2588 | C | GLU | 333 | 26.844 | 39.586 | 99.490 | 1.00 | 35.01 | AAGL |
| ATOM | 2589 | O | GLU | 333 | 27.924 | 40.109 | 99.776 | 1.00 | 33.69 | AAGL |
| ATOM | 2590 | N | LEU | 334 | 25.925 | 39.319 | 100.410 | 1.00 | 34.35 | AAGL |
| ATOM | 2591 | CA | LEU | 334 | 26.193 | 39.655 | 101.805 | 1.00 | 33.87 | AAGL |
| ATOM | 2592 | CB | LEU | 334 | 24.963 | 39.371 | 102.672 | 1.00 | 33.01 | AAGL |
| ATOM | 2593 | CG | LEU | 334 | 23.721 | 40.228 | 102.407 | 1.00 | 32.82 | AAGL |
| ATOM | 2594 | CD1 | LEU | 334 | 22.611 | 39.797 | 103.347 | 1.00 | 28.38 | AAGL |
| ATOM | 2595 | CD2 | LEU | 334 | 24.044 | 41.711 | 102.607 | 1.00 | 30.26 | AAGL |
| ATOM | 2596 | C | LEU | 334 | 27.396 | 38.881 | 102.344 | 1.00 | 35.69 | AAGL |
| ATOM | 2597 | O | LEU | 334 | 27.475 | 37.650 | 102.129 | 1.00 | 36.26 | AAGL |
| ATOM | 2598 | OXT | LEU | 334 | 28.249 | 39.520 | 102.989 | 1.00 | 35.77 | AAGL |
| END | | | | | | | | | | |

# Fig. 3 cont.

| HEADER | | | | | | | | | | BLGL |
|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1 | C | GLY | 11 | 35.975 | 14.251 | 23.684 | 1.00 | 48.49 | BLGL |
| ATOM | 2 | O | GLY | 11 | 36.590 | 13.193 | 23.517 | 1.00 | 48.50 | BLGL |
| ATOM | 3 | N | GLY | 11 | 36.372 | 16.222 | 25.216 | 1.00 | 48.08 | BLGL |
| ATOM | 4 | CA | GLY | 11 | 36.733 | 15.548 | 23.933 | 1.00 | 47.57 | BLGL |
| ATOM | 5 | N | LEU | 12 | 34.642 | 14.326 | 23.653 | 1.00 | 48.44 | BLGL |
| ATOM | 6 | CA | LEU | 12 | 33.796 | 13.147 | 23.416 | 1.00 | 45.49 | BLGL |
| ATOM | 7 | CB | LEU | 12 | 32.592 | 13.139 | 24.371 | 1.00 | 43.64 | BLGL |
| ATOM | 8 | CG | LEU | 12 | 31.626 | 11.961 | 24.199 | 1.00 | 41.45 | BLGL |
| ATOM | 9 | CD1 | LEU | 12 | 32.074 | 10.803 | 25.085 | 1.00 | 36.51 | BLGL |
| ATOM | 10 | CD2 | LEU | 12 | 30.203 | 12.400 | 24.550 | 1.00 | 41.11 | BLGL |
| ATOM | 11 | C | LEU | 12 | 33.272 | 13.109 | 21.979 | 1.00 | 44.11 | BLGL |
| ATOM | 12 | O | LEU | 12 | 32.688 | 14.086 | 21.502 | 1.00 | 45.18 | BLGL |
| ATOM | 13 | N | TYR | 13 | 33.487 | 11.986 | 21.295 | 1.00 | 42.63 | BLGL |
| ATOM | 14 | CA | TYR | 13 | 33.004 | 11.817 | 19.928 | 1.00 | 41.19 | BLGL |
| ATOM | 15 | CB | TYR | 13 | 34.083 | 11.206 | 19.042 | 1.00 | 45.36 | BLGL |
| ATOM | 16 | CG | TYR | 13 | 33.594 | 10.996 | 17.624 | 1.00 | 52.03 | BLGL |
| ATOM | 17 | CD1 | TYR | 13 | 33.232 | 9.727 | 17.167 | 1.00 | 53.91 | BLGL |
| ATOM | 18 | CE1 | TYR | 13 | 32.703 | 9.545 | 15.872 | 1.00 | 55.69 | BLGL |
| ATOM | 19 | CD2 | TYR | 13 | 33.420 | 12.083 | 16.756 | 1.00 | 53.77 | BLGL |
| ATOM | 20 | CE2 | TYR | 13 | 32.890 | 11.914 | 15.466 | 1.00 | 54.66 | BLGL |
| ATOM | 21 | CZ | TYR | 13 | 32.534 | 10.644 | 15.031 | 1.00 | 56.09 | BLGL |
| ATOM | 22 | OH | TYR | 13 | 32.009 | 10.473 | 13.764 | 1.00 | 56.62 | BLGL |
| ATOM | 23 | C | TYR | 13 | 31.755 | 10.932 | 19.837 | 1.00 | 38.22 | BLGL |
| ATOM | 24 | O | TYR | 13 | 31.686 | 9.887 | 20.471 | 1.00 | 38.74 | BLGL |
| ATOM | 25 | N | VAL | 14 | 30.776 | 11.355 | 19.039 | 1.00 | 34.88 | BLGL |
| ATOM | 26 | CA | VAL | 14 | 29.537 | 10.604 | 18.845 | 1.00 | 31.50 | BLGL |
| ATOM | 27 | CB | VAL | 14 | 28.418 | 11.094 | 19.777 | 1.00 | 30.78 | BLGL |
| ATOM | 28 | CG1 | VAL | 14 | 27.102 | 10.405 | 19.427 | 1.00 | 30.71 | BLGL |
| ATOM | 29 | CG2 | VAL | 14 | 28.790 | 10.812 | 21.203 | 1.00 | 30.70 | BLGL |
| ATOM | 30 | C | VAL | 14 | 29.069 | 10.798 | 17.420 | 1.00 | 30.74 | BLGL |
| ATOM | 31 | O | VAL | 14 | 28.776 | 11.917 | 17.007 | 1.00 | 31.52 | BLGL |
| ATOM | 32 | N | GLU | 15 | 28.994 | 9.710 | 16.669 | 1.00 | 30.21 | BLGL |
| ATOM | 33 | CA | GLU | 15 | 28.555 | 9.788 | 15.288 | 1.00 | 30.31 | BLGL |
| ATOM | 34 | CB | GLU | 15 | 29.002 | 8.546 | 14.534 | 1.00 | 33.96 | BLGL |
| ATOM | 35 | CG | GLU | 15 | 28.509 | 8.486 | 13.113 | 1.00 | 43.05 | BLGL |
| ATOM | 36 | CD | GLU | 15 | 28.927 | 7.202 | 12.424 | 1.00 | 49.32 | BLGL |
| ATOM | 37 | OE1 | GLU | 15 | 28.886 | 6.140 | 13.087 | 1.00 | 51.29 | BLGL |
| ATOM | 38 | OE2 | GLU | 15 | 29.285 | 7.251 | 11.223 | 1.00 | 54.28 | BLGL |
| ATOM | 39 | C | GLU | 15 | 27.045 | 9.931 | 15.206 | 1.00 | 28.83 | BLGL |
| ATOM | 40 | O | GLU | 15 | 26.303 | 9.161 | 15.816 | 1.00 | 26.88 | BLGL |
| ATOM | 41 | N | LYS | 16 | 26.596 | 10.923 | 14.445 | 1.00 | 29.24 | BLGL |
| ATOM | 42 | CA | LYS | 16 | 25.173 | 11.173 | 14.280 | 1.00 | 30.57 | BLGL |
| ATOM | 43 | CB | LYS | 16 | 24.933 | 12.207 | 13.174 | 1.00 | 32.52 | BLGL |
| ATOM | 44 | CG | LYS | 16 | 23.454 | 12.496 | 12.948 | 1.00 | 38.94 | BLGL |
| ATOM | 45 | CD | LYS | 16 | 23.141 | 12.889 | 11.510 | 1.00 | 43.38 | BLGL |
| ATOM | 46 | CE | LYS | 16 | 23.632 | 14.282 | 11.176 | 1.00 | 46.85 | BLGL |
| ATOM | 47 | NZ | LYS | 16 | 23.276 | 14.648 | 9.776 | 1.00 | 50.40 | BLGL |
| ATOM | 48 | C | LYS | 16 | 24.399 | 9.902 | 13.938 | 1.00 | 29.87 | BLGL |
| ATOM | 49 | O | LYS | 16 | 24.836 | 9.090 | 13.121 | 1.00 | 28.75 | BLGL |
| ATOM | 50 | N | VAL | 17 | 23.249 | 9.733 | 14.575 | 1.00 | 29.36 | BLGL |
| ATOM | 51 | CA | VAL | 17 | 22.394 | 8.591 | 14.306 | 1.00 | 29.25 | BLGL |
| ATOM | 52 | CB | VAL | 17 | 21.437 | 8.328 | 15.476 | 1.00 | 28.63 | BLGL |
| ATOM | 53 | CG1 | VAL | 17 | 20.469 | 7.201 | 15.127 | 1.00 | 28.74 | BLGL |
| ATOM | 54 | CG2 | VAL | 17 | 22.236 | 7.982 | 16.702 | 1.00 | 30.70 | BLGL |
| ATOM | 55 | C | VAL | 17 | 21.582 | 8.940 | 13.064 | 1.00 | 30.63 | BLGL |
| ATOM | 56 | O | VAL | 17 | 20.794 | 9.891 | 13.064 | 1.00 | 30.98 | BLGL |
| ATOM | 57 | N | SER | 18 | 21.782 | 8.172 | 12.005 | 1.00 | 30.58 | BLGL |
| ATOM | 58 | CA | SER | 18 | 21.083 | 8.422 | 10.758 | 1.00 | 33.73 | BLGL |
| ATOM | 59 | CB | SER | 18 | 21.787 | 7.675 | 9.628 | 1.00 | 36.18 | BLGL |
| ATOM | 60 | OG | SER | 18 | 21.984 | 6.324 | 9.990 | 1.00 | 38.96 | BLGL |
| ATOM | 61 | C | SER | 18 | 19.611 | 8.032 | 10.800 | 1.00 | 32.04 | BLGL |
| ATOM | 62 | O | SER | 18 | 19.264 | 6.933 | 11.231 | 1.00 | 31.91 | BLGL |
| ATOM | 63 | N | GLY | 19 | 18.755 | 8.950 | 10.359 | 1.00 | 31.92 | BLGL |
| ATOM | 64 | CA | GLY | 19 | 17.328 | 8.697 | 10.327 | 1.00 | 30.75 | BLGL |
| ATOM | 65 | C | GLY | 19 | 16.601 | 8.894 | 11.638 | 1.00 | 30.09 | BLGL |

# Fig. 4

| ATOM | 66  | O   | GLY | 19 | 15.395 | 8.684  | 11.705 | 1.00 | 32.49 | BLGL |
|------|-----|-----|-----|----|--------|--------|--------|------|-------|------|
| ATOM | 67  | N   | LEU | 20 | 17.314 | 9.295  | 12.681 | 1.00 | 28.46 | BLGL |
| ATOM | 68  | CA  | LEU | 20 | 16.672 | 9.498  | 13.967 | 1.00 | 28.28 | BLGL |
| ATOM | 69  | CB  | LEU | 20 | 17.706 | 9.910  | 15.013 | 1.00 | 29.28 | BLGL |
| ATOM | 70  | CG  | LEU | 20 | 17.141 | 9.983  | 16.436 | 1.00 | 29.10 | BLGL |
| ATOM | 71  | CD1 | LEU | 20 | 16.756 | 8.586  | 16.904 | 1.00 | 27.36 | BLGL |
| ATOM | 72  | CD2 | LEU | 20 | 18.165 | 10.598 | 17.359 | 1.00 | 29.58 | BLGL |
| ATOM | 73  | C   | LEU | 20 | 15.565 | 10.548 | 13.890 | 1.00 | 25.87 | BLGL |
| ATOM | 74  | O   | LEU | 20 | 15.821 | 11.686 | 13.535 | 1.00 | 24.28 | BLGL |
| ATOM | 75  | N   | ARG | 21 | 14.342 | 10.147 | 14.226 | 1.00 | 28.07 | BLGL |
| ATOM | 76  | CA  | ARG | 21 | 13.176 | 11.030 | 14.213 | 1.00 | 30.64 | BLGL |
| ATOM | 77  | CB  | ARG | 21 | 11.912 | 10.211 | 14.476 | 1.00 | 31.64 | BLGL |
| ATOM | 78  | CG  | ARG | 21 | 11.955 | 9.430  | 15.792 | 1.00 | 35.81 | BLGL |
| ATOM | 79  | CD  | ARG | 21 | 10.892 | 8.339  | 15.840 | 1.00 | 36.79 | BLGL |
| ATOM | 80  | NE  | ARG | 21 | 9.536  | 8.877  | 15.850 | 1.00 | 37.50 | BLGL |
| ATOM | 81  | CZ  | ARG | 21 | 8.445  | 8.133  | 15.699 | 1.00 | 38.47 | BLGL |
| ATOM | 82  | NH1 | ARG | 21 | 8.567  | 6.826  | 15.525 | 1.00 | 37.04 | BLGL |
| ATOM | 83  | NH2 | ARG | 21 | 7.235  | 8.688  | 15.731 | 1.00 | 39.56 | BLGL |
| ATOM | 84  | C   | ARG | 21 | 13.316 | 12.114 | 15.277 | 1.00 | 32.05 | BLGL |
| ATOM | 85  | O   | ARG | 21 | 13.840 | 11.862 | 16.354 | 1.00 | 31.41 | BLGL |
| ATOM | 86  | N   | LYS | 22 | 12.832 | 13.315 | 14.978 | 1.00 | 35.57 | BLGL |
| ATOM | 87  | CA  | LYS | 22 | 12.927 | 14.428 | 15.916 | 1.00 | 37.84 | BLGL |
| ATOM | 88  | CB  | LYS | 22 | 12.378 | 15.713 | 15.291 | 1.00 | 42.04 | BLGL |
| ATOM | 89  | CG  | LYS | 22 | 13.278 | 16.381 | 14.265 | 1.00 | 47.84 | BLGL |
| ATOM | 90  | CD  | LYS | 22 | 12.908 | 17.872 | 14.150 | 1.00 | 51.73 | BLGL |
| ATOM | 91  | CE  | LYS | 22 | 13.460 | 18.518 | 12.882 | 1.00 | 52.80 | BLGL |
| ATOM | 92  | NZ  | LYS | 22 | 12.732 | 18.062 | 11.661 | 1.00 | 52.64 | BLGL |
| ATOM | 93  | C   | LYS | 22 | 12.225 | 14.227 | 17.253 | 1.00 | 36.42 | BLGL |
| ATOM | 94  | O   | LYS | 22 | 12.672 | 14.762 | 18.264 | 1.00 | 37.54 | BLGL |
| ATOM | 95  | N   | ASP | 23 | 11.128 | 13.476 | 17.262 | 1.00 | 34.94 | BLGL |
| ATOM | 96  | CA  | ASP | 23 | 10.370 | 13.264 | 18.495 | 1.00 | 33.91 | BLGL |
| ATOM | 97  | CB  | ASP | 23 | 8.869  | 13.257 | 18.181 | 1.00 | 34.54 | BLGL |
| ATOM | 98  | CG  | ASP | 23 | 8.465  | 12.096 | 17.303 | 1.00 | 34.79 | BLGL |
| ATOM | 99  | OD1 | ASP | 23 | 9.242  | 11.739 | 16.392 | 1.00 | 33.67 | BLGL |
| ATOM | 100 | OD2 | ASP | 23 | 7.365  | 11.547 | 17.521 | 1.00 | 39.44 | BLGL |
| ATOM | 101 | C   | ASP | 23 | 10.754 | 11.989 | 19.238 | 1.00 | 31.78 | BLGL |
| ATOM | 102 | O   | ASP | 23 | 10.001 | 11.495 | 20.083 | 1.00 | 31.40 | BLGL |
| ATOM | 103 | N   | PHE | 24 | 11.932 | 11.467 | 18.921 | 1.00 | 28.21 | BLGL |
| ATOM | 104 | CA  | PHE | 24 | 12.423 | 10.256 | 19.551 | 1.00 | 25.65 | BLGL |
| ATOM | 105 | CB  | PHE | 24 | 13.788 | 9.904  | 18.967 | 1.00 | 25.73 | BLGL |
| ATOM | 106 | CG  | PHE | 24 | 14.281 | 8.538  | 19.337 | 1.00 | 25.81 | BLGL |
| ATOM | 107 | CD1 | PHE | 24 | 15.134 | 8.359  | 20.422 | 1.00 | 25.77 | BLGL |
| ATOM | 108 | CD2 | PHE | 24 | 13.930 | 7.431  | 18.573 | 1.00 | 25.98 | BLGL |
| ATOM | 109 | CE1 | PHE | 24 | 15.642 | 7.093  | 20.739 | 1.00 | 25.74 | BLGL |
| ATOM | 110 | CE2 | PHE | 24 | 14.431 | 6.161  | 18.881 | 1.00 | 27.08 | BLGL |
| ATOM | 111 | CZ  | PHE | 24 | 15.292 | 5.992  | 19.967 | 1.00 | 24.69 | BLGL |
| ATOM | 112 | C   | PHE | 24 | 12.517 | 10.473 | 21.055 | 1.00 | 22.99 | BLGL |
| ATOM | 113 | O   | PHE | 24 | 12.961 | 11.520 | 21.519 | 1.00 | 23.30 | BLGL |
| ATOM | 114 | N   | ILE | 25 | 12.077 | 9.474  | 21.804 | 1.00 | 19.49 | BLGL |
| ATOM | 115 | CA  | ILE | 25 | 12.096 | 9.514  | 23.254 | 1.00 | 17.47 | BLGL |
| ATOM | 116 | CB  | ILE | 25 | 11.137 | 8.465  | 23.820 | 1.00 | 15.37 | BLGL |
| ATOM | 117 | CG2 | ILE | 25 | 11.388 | 8.253  | 25.306 | 1.00 | 13.70 | BLGL |
| ATOM | 118 | CG1 | ILE | 25 | 9.706  | 8.883  | 23.524 | 1.00 | 13.77 | BLGL |
| ATOM | 119 | CD1 | ILE | 25 | 8.696  | 7.834  | 23.915 | 1.00 | 18.01 | BLGL |
| ATOM | 120 | C   | ILE | 25 | 13.487 | 9.227  | 23.799 | 1.00 | 17.49 | BLGL |
| ATOM | 121 | O   | ILE | 25 | 14.091 | 8.211  | 23.465 | 1.00 | 16.53 | BLGL |
| ATOM | 122 | N   | LYS | 26 | 13.985 | 10.128 | 24.637 | 1.00 | 16.78 | BLGL |
| ATOM | 123 | CA  | LYS | 26 | 15.294 | 9.962  | 25.259 | 1.00 | 18.11 | BLGL |
| ATOM | 124 | CB  | LYS | 26 | 16.213 | 11.096 | 24.825 | 1.00 | 19.07 | BLGL |
| ATOM | 125 | CG  | LYS | 26 | 16.276 | 11.237 | 23.314 | 1.00 | 21.25 | BLGL |
| ATOM | 126 | CD  | LYS | 26 | 16.943 | 12.520 | 22.899 | 1.00 | 23.74 | BLGL |
| ATOM | 127 | CE  | LYS | 26 | 16.949 | 12.669 | 21.387 | 1.00 | 24.53 | BLGL |
| ATOM | 128 | NZ  | LYS | 26 | 17.505 | 13.994 | 20.995 | 1.00 | 26.16 | BLGL |
| ATOM | 129 | C   | LYS | 26 | 15.032 | 10.015 | 26.754 | 1.00 | 17.62 | BLGL |
| ATOM | 130 | O   | LYS | 26 | 14.990 | 11.089 | 27.340 | 1.00 | 18.88 | BLGL |
| ATOM | 131 | N   | GLY | 27 | 14.845 | 8.850  | 27.367 | 1.00 | 15.97 | BLGL |

# Fig. 4 cont.

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 132 | CA | GLY | 27 | 14.540 | 8.822 | 28.783 | 1.00 | 14.87 | BLGL |
| ATOM | 133 | C | GLY | 27 | 15.553 | 8.183 | 29.706 | 1.00 | 15.36 | BLGL |
| ATOM | 134 | O | GLY | 27 | 16.490 | 7.523 | 29.278 | 1.00 | 14.26 | BLGL |
| ATOM | 135 | N | VAL | 28 | 15.364 | 8.413 | 30.997 | 1.00 | 15.73 | BLGL |
| ATOM | 136 | CA | VAL | 28 | 16.233 | 7.847 | 32.002 | 1.00 | 15.81 | BLGL |
| ATOM | 137 | CB | VAL | 28 | 17.285 | 8.866 | 32.505 | 1.00 | 15.33 | BLGL |
| ATOM | 138 | CG1 | VAL | 28 | 18.189 | 9.289 | 31.359 | 1.00 | 15.90 | BLGL |
| ATOM | 139 | CG2 | VAL | 28 | 16.604 | 10.073 | 33.113 | 1.00 | 15.60 | BLGL |
| ATOM | 140 | C | VAL | 28 | 15.367 | 7.411 | 33.164 | 1.00 | 17.23 | BLGL |
| ATOM | 141 | O | VAL | 28 | 14.294 | 7.967 | 33.405 | 1.00 | 16.45 | BLGL |
| ATOM | 142 | N | ASP | 29 | 15.817 | 6.380 | 33.860 | 1.00 | 17.41 | BLGL |
| ATOM | 143 | CA | ASP | 29 | 15.098 | 5.902 | 35.023 | 1.00 | 18.06 | BLGL |
| ATOM | 144 | CB | ASP | 29 | 14.855 | 4.391 | 34.925 | 1.00 | 16.28 | BLGL |
| ATOM | 145 | CG | ASP | 29 | 14.123 | 3.832 | 36.138 | 1.00 | 18.27 | BLGL |
| ATOM | 146 | OD1 | ASP | 29 | 13.426 | 2.801 | 35.978 | 1.00 | 15.84 | BLGL |
| ATOM | 147 | OD2 | ASP | 29 | 14.258 | 4.409 | 37.246 | 1.00 | 14.09 | BLGL |
| ATOM | 148 | C | ASP | 29 | 16.006 | 6.248 | 36.201 | 1.00 | 17.72 | BLGL |
| ATOM | 149 | O | ASP | 29 | 17.075 | 5.670 | 36.362 | 1.00 | 18.18 | BLGL |
| ATOM | 150 | N | VAL | 30 | 15.592 | 7.228 | 36.994 | 1.00 | 17.06 | BLGL |
| ATOM | 151 | CA | VAL | 30 | 16.360 | 7.653 | 38.158 | 1.00 | 14.73 | BLGL |
| ATOM | 152 | CB | VAL | 30 | 16.740 | 9.151 | 38.051 | 1.00 | 13.70 | BLGL |
| ATOM | 153 | CG1 | VAL | 30 | 17.688 | 9.354 | 36.880 | 1.00 | 12.16 | BLGL |
| ATOM | 154 | CG2 | VAL | 30 | 15.485 | 10.017 | 37.872 | 1.00 | 9.08 | BLGL |
| ATOM | 155 | C | VAL | 30 | 15.551 | 7.422 | 39.426 | 1.00 | 14.73 | BLGL |
| ATOM | 156 | O | VAL | 30 | 15.491 | 8.275 | 40.302 | 1.00 | 16.61 | BLGL |
| ATOM | 157 | N | SER | 31 | 14.931 | 6.252 | 39.515 | 1.00 | 16.06 | BLGL |
| ATOM | 158 | CA | SER | 31 | 14.090 | 5.899 | 40.660 | 1.00 | 19.01 | BLGL |
| ATOM | 159 | CB | SER | 31 | 13.540 | 4.481 | 40.481 | 1.00 | 17.38 | BLGL |
| ATOM | 160 | OG | SER | 31 | 12.719 | 4.395 | 39.331 | 1.00 | 19.20 | BLGL |
| ATOM | 161 | C | SER | 31 | 14.769 | 6.007 | 42.030 | 1.00 | 19.31 | BLGL |
| ATOM | 162 | O | SER | 31 | 14.120 | 6.282 | 43.041 | 1.00 | 19.82 | BLGL |
| ATOM | 163 | N | SER | 32 | 16.075 | 5.797 | 42.059 | 1.00 | 18.54 | BLGL |
| ATOM | 164 | CA | SER | 32 | 16.826 | 5.845 | 43.301 | 1.00 | 19.36 | BLGL |
| ATOM | 165 | CB | SER | 32 | 18.121 | 5.055 | 43.133 | 1.00 | 18.42 | BLGL |
| ATOM | 166 | OG | SER | 32 | 18.909 | 5.611 | 42.088 | 1.00 | 16.54 | BLGL |
| ATOM | 167 | C | SER | 32 | 17.161 | 7.259 | 43.775 | 1.00 | 21.13 | BLGL |
| ATOM | 168 | O | SER | 32 | 17.612 | 7.442 | 44.902 | 1.00 | 20.54 | BLGL |
| ATOM | 169 | N | ILE | 33 | 16.931 | 8.256 | 42.925 | 1.00 | 21.96 | BLGL |
| ATOM | 170 | CA | ILE | 33 | 17.256 | 9.644 | 43.263 | 1.00 | 22.33 | BLGL |
| ATOM | 171 | CB | ILE | 33 | 16.752 | 10.622 | 42.161 | 1.00 | 21.13 | BLGL |
| ATOM | 172 | CG2 | ILE | 33 | 15.234 | 10.621 | 42.095 | 1.00 | 19.56 | BLGL |
| ATOM | 173 | CG1 | ILE | 33 | 17.283 | 12.027 | 42.439 | 1.00 | 20.03 | BLGL |
| ATOM | 174 | CD1 | ILE | 33 | 18.794 | 12.117 | 42.425 | 1.00 | 17.45 | BLGL |
| ATOM | 175 | C | ILE | 33 | 16.796 | 10.152 | 44.636 | 1.00 | 23.71 | BLGL |
| ATOM | 176 | O | ILE | 33 | 17.549 | 10.858 | 45.309 | 1.00 | 25.43 | BLGL |
| ATOM | 177 | N | ILE | 34 | 15.581 | 9.797 | 45.059 | 1.00 | 24.35 | BLGL |
| ATOM | 178 | CA | ILE | 34 | 15.066 | 10.235 | 46.362 | 1.00 | 23.98 | BLGL |
| ATOM | 179 | CB | ILE | 34 | 13.539 | 9.951 | 46.486 | 1.00 | 23.20 | BLGL |
| ATOM | 180 | CG2 | ILE | 34 | 13.170 | 9.637 | 47.922 | 1.00 | 24.75 | BLGL |
| ATOM | 181 | CG1 | ILE | 34 | 12.735 | 11.183 | 46.063 | 1.00 | 20.84 | BLGL |
| ATOM | 182 | CD1 | ILE | 34 | 13.078 | 11.696 | 44.729 | 1.00 | 21.81 | BLGL |
| ATOM | 183 | C | ILE | 34 | 15.815 | 9.598 | 47.550 | 1.00 | 24.38 | BLGL |
| ATOM | 184 | O | ILE | 34 | 16.186 | 10.290 | 48.502 | 1.00 | 25.31 | BLGL |
| ATOM | 185 | N | ALA | 35 | 16.041 | 8.290 | 47.500 | 1.00 | 22.66 | BLGL |
| ATOM | 186 | CA | ALA | 35 | 16.761 | 7.622 | 48.579 | 1.00 | 22.83 | BLGL |
| ATOM | 187 | CB | ALA | 35 | 16.803 | 6.117 | 48.344 | 1.00 | 20.64 | BLGL |
| ATOM | 188 | C | ALA | 35 | 18.178 | 8.165 | 48.681 | 1.00 | 23.42 | BLGL |
| ATOM | 189 | O | ALA | 35 | 18.687 | 8.377 | 49.776 | 1.00 | 25.98 | BLGL |
| ATOM | 190 | N | LEU | 36 | 18.813 | 8.382 | 47.536 | 1.00 | 23.28 | BLGL |
| ATOM | 191 | CA | LEU | 36 | 20.173 | 8.900 | 47.508 | 1.00 | 25.90 | BLGL |
| ATOM | 192 | CB | LEU | 36 | 20.726 | 8.908 | 46.073 | 1.00 | 26.42 | BLGL |
| ATOM | 193 | CG | LEU | 36 | 21.093 | 7.571 | 45.421 | 1.00 | 25.94 | BLGL |
| ATOM | 194 | CD1 | LEU | 36 | 21.783 | 7.836 | 44.105 | 1.00 | 29.58 | BLGL |
| ATOM | 195 | CD2 | LEU | 36 | 22.017 | 6.778 | 46.323 | 1.00 | 28.67 | BLGL |
| ATOM | 196 | C | LEU | 36 | 20.237 | 10.308 | 48.089 | 1.00 | 26.59 | BLGL |
| ATOM | 197 | O | LEU | 36 | 21.140 | 10.637 | 48.863 | 1.00 | 25.84 | BLGL |

**Fig. 4 cont.**

| ATOM | 198 | N | GLU | 37 | 19.282 | 11.144 | 47.708 | 1.00 | 26.12 | BLGL |
|------|-----|------|-----|----|--------|--------|--------|------|-------|------|
| ATOM | 199 | CA | GLU | 37 | 19.259 | 12.501 | 48.214 | 1.00 | 28.35 | BLGL |
| ATOM | 200 | CB | GLU | 37 | 18.092 | 13.264 | 47.594 | 1.00 | 26.08 | BLGL |
| ATOM | 201 | CG | GLU | 37 | 18.409 | 13.814 | 46.220 | 1.00 | 29.12 | BLGL |
| ATOM | 202 | CD | GLU | 37 | 17.238 | 14.542 | 45.612 | 1.00 | 30.50 | BLGL |
| ATOM | 203 | OE1 | GLU | 37 | 17.422 | 15.243 | 44.593 | 1.00 | 26.60 | BLGL |
| ATOM | 204 | OE2 | GLU | 37 | 16.128 | 14.400 | 46.163 | 1.00 | 35.60 | BLGL |
| ATOM | 205 | C | GLU | 37 | 19.170 | 12.526 | 49.739 | 1.00 | 28.90 | BLGL |
| ATOM | 206 | O | GLU | 37 | 19.828 | 13.334 | 50.393 | 1.00 | 30.03 | BLGL |
| ATOM | 207 | N | GLU | 38 | 18.366 | 11.633 | 50.301 | 1.00 | 29.70 | BLGL |
| ATOM | 208 | CA | GLU | 38 | 18.212 | 11.570 | 51.746 | 1.00 | 31.72 | BLGL |
| ATOM | 209 | CB | GLU | 38 | 17.037 | 10.677 | 52.125 | 1.00 | 31.95 | BLGL |
| ATOM | 210 | CG | GLU | 38 | 15.752 | 11.052 | 51.450 | 1.00 | 37.83 | BLGL |
| ATOM | 211 | CD | GLU | 38 | 14.562 | 10.379 | 52.094 | 1.00 | 40.58 | BLGL |
| ATOM | 212 | OE1 | GLU | 38 | 14.609 | 9.150 | 52.302 | 1.00 | 39.84 | BLGL |
| ATOM | 213 | OE2 | GLU | 38 | 13.578 | 11.086 | 52.390 | 1.00 | 45.75 | BLGL |
| ATOM | 214 | C | GLU | 38 | 19.467 | 11.026 | 52.415 | 1.00 | 32.56 | BLGL |
| ATOM | 215 | O | GLU | 38 | 19.641 | 11.156 | 53.627 | 1.00 | 36.26 | BLGL |
| ATOM | 216 | N | SER | 39 | 20.335 | 10.402 | 51.632 | 1.00 | 30.07 | BLGL |
| ATOM | 217 | CA | SER | 39 | 21.553 | 9.842 | 52.176 | 1.00 | 27.49 | BLGL |
| ATOM | 218 | CB | SER | 39 | 21.939 | 8.602 | 51.379 | 1.00 | 29.09 | BLGL |
| ATOM | 219 | OG | SER | 39 | 20.872 | 7.667 | 51.376 | 1.00 | 24.83 | BLGL |
| ATOM | 220 | C | SER | 39 | 22.660 | 10.882 | 52.133 | 1.00 | 28.20 | BLGL |
| ATOM | 221 | O | SER | 39 | 23.791 | 10.624 | 52.547 | 1.00 | 29.82 | BLGL |
| ATOM | 222 | N | GLY | 40 | 22.327 | 12.063 | 51.626 | 1.00 | 28.31 | BLGL |
| ATOM | 223 | CA | GLY | 40 | 23.303 | 13.135 | 51.558 | 1.00 | 29.30 | BLGL |
| ATOM | 224 | C | GLY | 40 | 23.975 | 13.332 | 50.214 | 1.00 | 29.65 | BLGL |
| ATOM | 225 | O | GLY | 40 | 24.717 | 14.296 | 50.031 | 1.00 | 31.52 | BLGL |
| ATOM | 226 | N | VAL | 41 | 23.730 | 12.428 | 49.272 | 1.00 | 28.29 | BLGL |
| ATOM | 227 | CA | VAL | 41 | 24.333 | 12.540 | 47.948 | 1.00 | 27.33 | BLGL |
| ATOM | 228 | CB | VAL | 41 | 24.014 | 11.299 | 47.075 | 1.00 | 26.80 | BLGL |
| ATOM | 229 | CG1 | VAL | 41 | 24.634 | 11.458 | 45.699 | 1.00 | 24.11 | BLGL |
| ATOM | 230 | CG2 | VAL | 41 | 24.531 | 10.034 | 47.754 | 1.00 | 25.53 | BLGL |
| ATOM | 231 | C | VAL | 41 | 23.816 | 13.788 | 47.242 | 1.00 | 27.51 | BLGL |
| ATOM | 232 | O | VAL | 41 | 22.630 | 14.107 | 47.315 | 1.00 | 27.71 | BLGL |
| ATOM | 233 | N | ALA | 42 | 24.716 | 14.496 | 46.568 | 1.00 | 28.05 | BLGL |
| ATOM | 234 | CA | ALA | 42 | 24.364 | 15.713 | 45.840 | 1.00 | 27.62 | BLGL |
| ATOM | 235 | CB | ALA | 42 | 24.952 | 16.935 | 46.538 | 1.00 | 26.85 | BLGL |
| ATOM | 236 | C | ALA | 42 | 24.898 | 15.624 | 44.415 | 1.00 | 28.00 | BLGL |
| ATOM | 237 | O | ALA | 42 | 25.918 | 14.986 | 44.158 | 1.00 | 29.09 | BLGL |
| ATOM | 238 | N | PHE | 43 | 24.205 | 16.267 | 43.489 | 1.00 | 27.56 | BLGL |
| ATOM | 239 | CA | PHE | 43 | 24.625 | 16.244 | 42.101 | 1.00 | 30.30 | BLGL |
| ATOM | 240 | CB | PHE | 43 | 23.529 | 15.626 | 41.223 | 1.00 | 29.43 | BLGL |
| ATOM | 241 | CG | PHE | 43 | 23.281 | 14.176 | 41.513 | 1.00 | 29.78 | BLGL |
| ATOM | 242 | CD1 | PHE | 43 | 22.538 | 13.791 | 42.630 | 1.00 | 26.98 | BLGL |
| ATOM | 243 | CD2 | PHE | 43 | 23.855 | 13.188 | 40.714 | 1.00 | 28.78 | BLGL |
| ATOM | 244 | CE1 | PHE | 43 | 22.373 | 12.442 | 42.957 | 1.00 | 25.96 | BLGL |
| ATOM | 245 | CE2 | PHE | 43 | 23.698 | 11.835 | 41.031 | 1.00 | 28.67 | BLGL |
| ATOM | 246 | CZ | PHE | 43 | 22.954 | 11.461 | 42.160 | 1.00 | 26.33 | BLGL |
| ATOM | 247 | C | PHE | 43 | 24.954 | 17.651 | 41.632 | 1.00 | 32.38 | BLGL |
| ATOM | 248 | O | PHE | 43 | 24.351 | 18.622 | 42.096 | 1.00 | 33.12 | BLGL |
| ATOM | 249 | N | TYR | 44 | 25.915 | 17.759 | 40.719 | 1.00 | 32.89 | BLGL |
| ATOM | 250 | CA | TYR | 44 | 26.326 | 19.054 | 40.203 | 1.00 | 34.23 | BLGL |
| ATOM | 251 | CB | TYR | 44 | 27.807 | 19.289 | 40.482 | 1.00 | 33.04 | BLGL |
| ATOM | 252 | CG | TYR | 44 | 28.165 | 19.083 | 41.926 | 1.00 | 33.71 | BLGL |
| ATOM | 253 | CD1 | TYR | 44 | 28.177 | 17.809 | 42.481 | 1.00 | 32.43 | BLGL |
| ATOM | 254 | CE1 | TYR | 44 | 28.453 | 17.617 | 43.820 | 1.00 | 35.78 | BLGL |
| ATOM | 255 | CD2 | TYR | 44 | 28.444 | 20.167 | 42.752 | 1.00 | 34.36 | BLGL |
| ATOM | 256 | CE2 | TYR | 44 | 28.721 | 19.986 | 44.099 | 1.00 | 34.85 | BLGL |
| ATOM | 257 | CZ | TYR | 44 | 28.722 | 18.708 | 44.627 | 1.00 | 35.70 | BLGL |
| ATOM | 258 | OH | TYR | 44 | 28.974 | 18.515 | 45.966 | 1.00 | 37.37 | BLGL |
| ATOM | 259 | C | TYR | 44 | 26.085 | 19.114 | 38.717 | 1.00 | 35.88 | BLGL |
| ATOM | 260 | O | TYR | 44 | 25.531 | 18.189 | 38.134 | 1.00 | 36.33 | BLGL |
| ATOM | 261 | N | ASN | 45 | 26.509 | 20.211 | 38.106 | 1.00 | 39.58 | BLGL |
| ATOM | 262 | CA | ASN | 45 | 26.350 | 20.391 | 36.672 | 1.00 | 43.09 | BLGL |
| ATOM | 263 | CB | ASN | 45 | 25.429 | 21.581 | 36.391 | 1.00 | 45.50 | BLGL |

# Fig. 4 cont.

| ATOM | 264 | CG | ASN | 45 | 26.156 | 22.912 | 36.452 | 1.00 | 47.10 | BLGL |
|------|-----|-----|-----|-----|--------|--------|--------|------|-------|------|
| ATOM | 265 | OD1 | ASN | 45 | 26.932 | 23.180 | 37.373 | 1.00 | 44.32 | BLGL |
| ATOM | 266 | ND2 | ASN | 45 | 25.897 | 23.760 | 35.464 | 1.00 | 49.84 | BLGL |
| ATOM | 267 | C | ASN | 45 | 27.721 | 20.618 | 36.038 | 1.00 | 43.53 | BLGL |
| ATOM | 268 | O | ASN | 45 | 28.746 | 20.564 | 36.718 | 1.00 | 41.75 | BLGL |
| ATOM | 269 | N | GLU | 46 | 27.733 | 20.861 | 34.735 | 1.00 | 47.02 | BLGL |
| ATOM | 270 | CA | GLU | 46 | 28.979 | 21.090 | 34.011 | 1.00 | 51.61 | BLGL |
| ATOM | 271 | CB | GLU | 46 | 28.673 | 21.715 | 32.656 | 1.00 | 55.53 | BLGL |
| ATOM | 272 | CG | GLU | 46 | 27.635 | 20.976 | 31.820 | 1.00 | 59.75 | BLGL |
| ATOM | 273 | CD | GLU | 46 | 28.162 | 19.673 | 31.261 | 1.00 | 62.26 | BLGL |
| ATOM | 274 | OE1 | GLU | 46 | 29.304 | 19.665 | 30.749 | 1.00 | 62.58 | BLGL |
| ATOM | 275 | OE2 | GLU | 46 | 27.429 | 18.665 | 31.320 | 1.00 | 63.83 | BLGL |
| ATOM | 276 | C | GLU | 46 | 29.917 | 22.027 | 34.782 | 1.00 | 52.77 | BLGL |
| ATOM | 277 | O | GLU | 46 | 31.035 | 21.648 | 35.144 | 1.00 | 52.27 | BLGL |
| ATOM | 278 | N | SER | 47 | 29.440 | 23.248 | 35.029 | 1.00 | 53.78 | BLGL |
| ATOM | 279 | CA | SER | 47 | 30.197 | 24.288 | 35.723 | 1.00 | 54.29 | BLGL |
| ATOM | 280 | CB | SER | 47 | 29.312 | 25.518 | 35.940 | 1.00 | 56.24 | BLGL |
| ATOM | 281 | OG | SER | 47 | 28.822 | 26.029 | 34.707 | 1.00 | 57.54 | BLGL |
| ATOM | 282 | C | SER | 47 | 30.779 | 23.857 | 37.058 | 1.00 | 54.34 | BLGL |
| ATOM | 283 | O | SER | 47 | 31.720 | 24.477 | 37.552 | 1.00 | 56.28 | BLGL |
| ATOM | 284 | N | GLY | 48 | 30.215 | 22.812 | 37.651 | 1.00 | 53.12 | BLGL |
| ATOM | 285 | CA | GLY | 48 | 30.724 | 22.344 | 38.926 | 1.00 | 52.44 | BLGL |
| ATOM | 286 | C | GLY | 48 | 29.883 | 22.783 | 40.109 | 1.00 | 52.32 | BLGL |
| ATOM | 287 | O | GLY | 48 | 30.200 | 22.455 | 41.258 | 1.00 | 51.88 | BLGL |
| ATOM | 288 | N | LYS | 49 | 28.807 | 23.518 | 39.832 | 1.00 | 51.68 | BLGL |
| ATOM | 289 | CA | LYS | 49 | 27.919 | 24.009 | 40.882 | 1.00 | 50.92 | BLGL |
| ATOM | 290 | CB | LYS | 49 | 27.338 | 25.368 | 40.477 | 1.00 | 52.51 | BLGL |
| ATOM | 291 | CG | LYS | 49 | 26.440 | 25.314 | 39.255 | 1.00 | 54.74 | BLGL |
| ATOM | 292 | CD | LYS | 49 | 26.139 | 26.704 | 38.706 | 1.00 | 58.30 | BLGL |
| ATOM | 293 | CE | LYS | 49 | 25.326 | 27.551 | 39.672 | 1.00 | 59.50 | BLGL |
| ATOM | 294 | NZ | LYS | 49 | 25.039 | 28.909 | 39.112 | 1.00 | 61.13 | BLGL |
| ATOM | 295 | C | LYS | 49 | 26.779 | 23.039 | 41.204 | 1.00 | 49.26 | BLGL |
| ATOM | 296 | O | LYS | 49 | 26.215 | 22.391 | 40.320 | 1.00 | 50.56 | BLGL |
| ATOM | 297 | N | LYS | 50 | 26.444 | 22.953 | 42.483 | 1.00 | 46.67 | BLGL |
| ATOM | 298 | CA | LYS | 50 | 25.377 | 22.082 | 42.955 | 1.00 | 44.89 | BLGL |
| ATOM | 299 | CB | LYS | 50 | 25.229 | 22.272 | 44.465 | 1.00 | 44.47 | BLGL |
| ATOM | 300 | CG | LYS | 50 | 24.483 | 21.182 | 45.190 | 1.00 | 47.37 | BLGL |
| ATOM | 301 | CD | LYS | 50 | 24.732 | 21.290 | 46.692 | 1.00 | 50.81 | BLGL |
| ATOM | 302 | CE | LYS | 50 | 23.926 | 20.260 | 47.478 | 1.00 | 53.40 | BLGL |
| ATOM | 303 | NZ | LYS | 50 | 24.326 | 20.203 | 48.917 | 1.00 | 55.24 | BLGL |
| ATOM | 304 | C | LYS | 50 | 24.088 | 22.473 | 42.221 | 1.00 | 43.33 | BLGL |
| ATOM | 305 | O | LYS | 50 | 23.726 | 23.647 | 42.187 | 1.00 | 43.90 | BLGL |
| ATOM | 306 | N | GLN | 51 | 23.400 | 21.497 | 41.631 | 1.00 | 41.68 | BLGL |
| ATOM | 307 | CA | GLN | 51 | 22.167 | 21.765 | 40.884 | 1.00 | 38.41 | BLGL |
| ATOM | 308 | CB | GLN | 51 | 22.531 | 22.164 | 39.449 | 1.00 | 38.23 | BLGL |
| ATOM | 309 | CG | GLN | 51 | 21.352 | 22.358 | 38.507 | 1.00 | 38.66 | BLGL |
| ATOM | 310 | CD | GLN | 51 | 21.797 | 22.731 | 37.099 | 1.00 | 38.67 | BLGL |
| ATOM | 311 | OE1 | GLN | 51 | 22.206 | 23.862 | 36.846 | 1.00 | 38.64 | BLGL |
| ATOM | 312 | NE2 | GLN | 51 | 21.730 | 21.771 | 36.181 | 1.00 | 38.86 | BLGL |
| ATOM | 313 | C | GLN | 51 | 21.241 | 20.548 | 40.867 | 1.00 | 35.96 | BLGL |
| ATOM | 314 | O | GLN | 51 | 21.714 | 19.417 | 40.893 | 1.00 | 35.98 | BLGL |
| ATOM | 315 | N | ASP | 52 | 19.928 | 20.778 | 40.827 | 1.00 | 34.78 | BLGL |
| ATOM | 316 | CA | ASP | 52 | 18.955 | 19.677 | 40.797 | 1.00 | 34.16 | BLGL |
| ATOM | 317 | CB | ASP | 52 | 17.522 | 20.215 | 40.657 | 1.00 | 35.75 | BLGL |
| ATOM | 318 | CG | ASP | 52 | 16.475 | 19.100 | 40.603 | 1.00 | 36.25 | BLGL |
| ATOM | 319 | OD1 | ASP | 52 | 15.271 | 19.396 | 40.465 | 1.00 | 35.18 | BLGL |
| ATOM | 320 | OD2 | ASP | 52 | 16.857 | 17.919 | 40.703 | 1.00 | 41.59 | BLGL |
| ATOM | 321 | C | ASP | 52 | 19.269 | 18.760 | 39.610 | 1.00 | 33.33 | BLGL |
| ATOM | 322 | O | ASP | 52 | 19.475 | 19.231 | 38.483 | 1.00 | 33.59 | BLGL |
| ATOM | 323 | N | ILE | 53 | 19.294 | 17.454 | 39.856 | 1.00 | 29.47 | BLGL |
| ATOM | 324 | CA | ILE | 53 | 19.620 | 16.512 | 38.797 | 1.00 | 26.79 | BLGL |
| ATOM | 325 | CB | ILE | 53 | 19.692 | 15.059 | 39.336 | 1.00 | 25.32 | BLGL |
| ATOM | 326 | CG2 | ILE | 53 | 18.304 | 14.567 | 39.715 | 1.00 | 24.80 | BLGL |
| ATOM | 327 | CG1 | ILE | 53 | 20.326 | 14.147 | 38.277 | 1.00 | 25.86 | BLGL |
| ATOM | 328 | CD1 | ILE | 53 | 20.638 | 12.753 | 38.777 | 1.00 | 25.81 | BLGL |
| ATOM | 329 | C | ILE | 53 | 18.644 | 16.588 | 37.631 | 1.00 | 25.41 | BLGL |

# Fig. 4 cont.

| ATOM | 330 | O | ILE | 53 | 19.042 | 16.436 | 36.475 | 1.00 | 23.70 | BLGL |
|------|-----|-----|-----|----|--------|--------|--------|------|-------|------|
| ATOM | 331 | N | PHE | 54 | 17.372 | 16.836 | 37.926 | 1.00 | 23.59 | BLGL |
| ATOM | 332 | CA | PHE | 54 | 16.380 | 16.930 | 36.868 | 1.00 | 25.83 | BLGL |
| ATOM | 333 | CB | PHE | 54 | 14.972 | 17.002 | 37.456 | 1.00 | 23.83 | BLGL |
| ATOM | 334 | CG | PHE | 54 | 14.526 | 15.723 | 38.072 | 1.00 | 22.74 | BLGL |
| ATOM | 335 | CD1 | PHE | 54 | 14.799 | 15.449 | 39.402 | 1.00 | 25.01 | BLGL |
| ATOM | 336 | CD2 | PHE | 54 | 13.885 | 14.760 | 37.306 | 1.00 | 21.32 | BLGL |
| ATOM | 337 | CE1 | PHE | 54 | 14.443 | 14.229 | 39.961 | 1.00 | 27.14 | BLGL |
| ATOM | 338 | CE2 | PHE | 54 | 13.525 | 13.537 | 37.856 | 1.00 | 23.72 | BLGL |
| ATOM | 339 | CZ | PHE | 54 | 13.803 | 13.268 | 39.184 | 1.00 | 24.12 | BLGL |
| ATOM | 340 | C | PHE | 54 | 16.641 | 18.121 | 35.953 | 1.00 | 27.75 | BLGL |
| ATOM | 341 | O | PHE | 54 | 16.378 | 18.064 | 34.753 | 1.00 | 27.66 | BLGL |
| ATOM | 342 | N | ASN | 55 | 17.167 | 19.197 | 36.522 | 1.00 | 30.60 | BLGL |
| ATOM | 343 | CA | ASN | 55 | 17.485 | 20.385 | 35.740 | 1.00 | 32.40 | BLGL |
| ATOM | 344 | CB | ASN | 55 | 17.927 | 21.528 | 36.665 | 1.00 | 38.72 | BLGL |
| ATOM | 345 | CG | ASN | 55 | 18.157 | 22.835 | 35.919 | 1.00 | 43.16 | BLGL |
| ATOM | 346 | OD1 | ASN | 55 | 18.775 | 23.767 | 36.444 | 1.00 | 46.30 | BLGL |
| ATOM | 347 | ND2 | ASN | 55 | 17.657 | 22.912 | 34.692 | 1.00 | 47.38 | BLGL |
| ATOM | 348 | C | ASN | 55 | 18.631 | 19.996 | 34.808 | 1.00 | 30.86 | BLGL |
| ATOM | 349 | O | ASN | 55 | 18.624 | 20.327 | 33.623 | 1.00 | 29.18 | BLGL |
| ATOM | 350 | N | THR | 56 | 19.608 | 19.281 | 35.363 | 1.00 | 28.42 | BLGL |
| ATOM | 351 | CA | THR | 56 | 20.765 | 18.824 | 34.606 | 1.00 | 26.82 | BLGL |
| ATOM | 352 | CB | THR | 56 | 21.769 | 18.101 | 35.514 | 1.00 | 27.58 | BLGL |
| ATOM | 353 | OG1 | THR | 56 | 22.198 | 18.988 | 36.558 | 1.00 | 29.47 | BLGL |
| ATOM | 354 | CG2 | THR | 56 | 22.969 | 17.642 | 34.714 | 1.00 | 22.45 | BLGL |
| ATOM | 355 | C | THR | 56 | 20.353 | 17.870 | 33.489 | 1.00 | 27.22 | BLGL |
| ATOM | 356 | O | THR | 56 | 20.851 | 17.952 | 32.366 | 1.00 | 27.23 | BLGL |
| ATOM | 357 | N | LEU | 57 | 19.441 | 16.961 | 33.805 | 1.00 | 27.52 | BLGL |
| ATOM | 358 | CA | LEU | 57 | 18.950 | 15.997 | 32.830 | 1.00 | 27.42 | BLGL |
| ATOM | 359 | CB | LEU | 57 | 17.978 | 15.033 | 33.508 | 1.00 | 26.87 | BLGL |
| ATOM | 360 | CG | LEU | 57 | 18.453 | 13.617 | 33.847 | 1.00 | 26.41 | BLGL |
| ATOM | 361 | CD1 | LEU | 57 | 19.941 | 13.572 | 34.078 | 1.00 | 23.65 | BLGL |
| ATOM | 362 | CD2 | LEU | 57 | 17.691 | 13.138 | 35.074 | 1.00 | 25.32 | BLGL |
| ATOM | 363 | C | LEU | 57 | 18.257 | 16.686 | 31.662 | 1.00 | 28.88 | BLGL |
| ATOM | 364 | O | LEU | 57 | 18.430 | 16.288 | 30.515 | 1.00 | 29.93 | BLGL |
| ATOM | 365 | N | LYS | 58 | 17.474 | 17.718 | 31.959 | 1.00 | 30.47 | BLGL |
| ATOM | 366 | CA | LYS | 58 | 16.757 | 18.455 | 30.926 | 1.00 | 30.56 | BLGL |
| ATOM | 367 | CB | LYS | 58 | 15.836 | 19.507 | 31.561 | 1.00 | 32.82 | BLGL |
| ATOM | 368 | CG | LYS | 58 | 15.038 | 20.330 | 30.551 | 1.00 | 33.72 | BLGL |
| ATOM | 369 | CD | LYS | 58 | 14.129 | 19.438 | 29.710 | 1.00 | 36.45 | BLGL |
| ATOM | 370 | CE | LYS | 58 | 13.279 | 20.253 | 28.732 | 1.00 | 38.35 | BLGL |
| ATOM | 371 | NZ | LYS | 58 | 12.233 | 19.436 | 28.049 | 1.00 | 36.51 | BLGL |
| ATOM | 372 | C | LYS | 58 | 17.726 | 19.135 | 29.969 | 1.00 | 30.23 | BLGL |
| ATOM | 373 | O | LYS | 58 | 17.564 | 19.064 | 28.753 | 1.00 | 31.14 | BLGL |
| ATOM | 374 | N | GLU | 59 | 18.734 | 19.793 | 30.522 | 1.00 | 30.65 | BLGL |
| ATOM | 375 | CA | GLU | 59 | 19.722 | 20.483 | 29.709 | 1.00 | 31.60 | BLGL |
| ATOM | 376 | CB | GLU | 59 | 20.668 | 21.275 | 30.610 | 1.00 | 35.74 | BLGL |
| ATOM | 377 | CG | GLU | 59 | 19.971 | 22.381 | 31.397 | 1.00 | 42.93 | BLGL |
| ATOM | 378 | CD | GLU | 59 | 20.839 | 22.960 | 32.511 | 1.00 | 48.75 | BLGL |
| ATOM | 379 | OE1 | GLU | 59 | 20.327 | 23.818 | 33.264 | 1.00 | 51.01 | BLGL |
| ATOM | 380 | OE2 | GLU | 59 | 22.026 | 22.558 | 32.638 | 1.00 | 51.49 | BLGL |
| ATOM | 381 | C | GLU | 59 | 20.511 | 19.493 | 28.862 | 1.00 | 30.47 | BLGL |
| ATOM | 382 | O | GLU | 59 | 21.086 | 19.859 | 27.838 | 1.00 | 30.17 | BLGL |
| ATOM | 383 | N | ALA | 60 | 20.531 | 18.235 | 29.293 | 1.00 | 29.36 | BLGL |
| ATOM | 384 | CA | ALA | 60 | 21.253 | 17.186 | 28.582 | 1.00 | 28.02 | BLGL |
| ATOM | 385 | CB | ALA | 60 | 21.611 | 16.065 | 29.543 | 1.00 | 29.83 | BLGL |
| ATOM | 386 | C | ALA | 60 | 20.461 | 16.623 | 27.406 | 1.00 | 27.47 | BLGL |
| ATOM | 387 | O | ALA | 60 | 20.975 | 15.807 | 26.643 | 1.00 | 26.82 | BLGL |
| ATOM | 388 | N | GLY | 61 | 19.208 | 17.048 | 27.269 | 1.00 | 27.12 | BLGL |
| ATOM | 389 | CA | GLY | 61 | 18.387 | 16.574 | 26.167 | 1.00 | 25.98 | BLGL |
| ATOM | 390 | C | GLY | 61 | 17.379 | 15.484 | 26.500 | 1.00 | 24.46 | BLGL |
| ATOM | 391 | O | GLY | 61 | 16.678 | 14.995 | 25.613 | 1.00 | 22.97 | BLGL |
| ATOM | 392 | N | VAL | 62 | 17.307 | 15.101 | 27.773 | 1.00 | 23.85 | BLGL |
| ATOM | 393 | CA | VAL | 62 | 16.373 | 14.075 | 28.223 | 1.00 | 22.41 | BLGL |
| ATOM | 394 | CB | VAL | 62 | 16.738 | 13.577 | 29.651 | 1.00 | 22.60 | BLGL |
| ATOM | 395 | CG1 | VAL | 62 | 15.754 | 12.514 | 30.107 | 1.00 | 22.01 | BLGL |

# Fig. 4 cont.

| ATOM | 396 | CG2 | VAL | 62 | 18.146 | 13.018 | 29.664 | 1.00 | 20.65 | BLGL |
|------|-----|-----|-----|----|--------|--------|--------|------|-------|------|
| ATOM | 397 | C | VAL | 62 | 14.958 | 14.658 | 28.230 | 1.00 | 22.28 | BLGL |
| ATOM | 398 | O | VAL | 62 | 14.743 | 15.783 | 28.686 | 1.00 | 24.37 | BLGL |
| ATOM | 399 | N | ASN | 63 | 13.997 | 13.896 | 27.721 | 1.00 | 20.64 | BLGL |
| ATOM | 400 | CA | ASN | 63 | 12.615 | 14.356 | 27.660 | 1.00 | 21.22 | BLGL |
| ATOM | 401 | CB | ASN | 63 | 12.203 | 14.546 | 26.204 | 1.00 | 20.41 | BLGL |
| ATOM | 402 | CG | ASN | 63 | 12.528 | 13.337 | 25.349 | 1.00 | 20.90 | BLGL |
| ATOM | 403 | OD1 | ASN | 63 | 12.248 | 12.195 | 25.723 | 1.00 | 22.33 | BLGL |
| ATOM | 404 | ND2 | ASN | 63 | 13.112 | 13.581 | 24.189 | 1.00 | 20.98 | BLGL |
| ATOM | 405 | C | ASN | 63 | 11.641 | 13.396 | 28.330 | 1.00 | 21.56 | BLGL |
| ATOM | 406 | O | ASN | 63 | 10.426 | 13.606 | 28.304 | 1.00 | 24.89 | BLGL |
| ATOM | 407 | N | TYR | 64 | 12.171 | 12.346 | 28.939 | 1.00 | 19.85 | BLGL |
| ATOM | 408 | CA | TYR | 64 | 11.323 | 11.360 | 29.578 | 1.00 | 18.37 | BLGL |
| ATOM | 409 | CB | TYR | 64 | 11.054 | 10.226 | 28.590 | 1.00 | 18.15 | BLGL |
| ATOM | 410 | CG | TYR | 64 | 9.601 | 10.025 | 28.244 | 1.00 | 18.02 | BLGL |
| ATOM | 411 | CD1 | TYR | 64 | 8.724 | 9.446 | 29.155 | 1.00 | 16.59 | BLGL |
| ATOM | 412 | CE1 | TYR | 64 | 7.397 | 9.210 | 28.821 | 1.00 | 17.75 | BLGL |
| ATOM | 413 | CD2 | TYR | 64 | 9.109 | 10.375 | 26.985 | 1.00 | 20.14 | BLGL |
| ATOM | 414 | CE2 | TYR | 64 | 7.781 | 10.145 | 26.640 | 1.00 | 17.07 | BLGL |
| ATOM | 415 | CZ | TYR | 64 | 6.935 | 9.560 | 27.562 | 1.00 | 18.10 | BLGL |
| ATOM | 416 | OH | TYR | 64 | 5.634 | 9.301 | 27.223 | 1.00 | 19.97 | BLGL |
| ATOM | 417 | C | TYR | 64 | 11.963 | 10.804 | 30.839 | 1.00 | 17.64 | BLGL |
| ATOM | 418 | O | TYR | 64 | 13.181 | 10.683 | 30.927 | 1.00 | 17.84 | BLGL |
| ATOM | 419 | N | VAL | 65 | 11.137 | 10.470 | 31.819 | 1.00 | 15.63 | BLGL |
| ATOM | 420 | CA | VAL | 65 | 11.644 | 9.905 | 33.050 | 1.00 | 16.50 | BLGL |
| ATOM | 421 | CB | VAL | 65 | 11.567 | 10.909 | 34.215 | 1.00 | 15.92 | BLGL |
| ATOM | 422 | CG1 | VAL | 65 | 11.909 | 10.207 | 35.522 | 1.00 | 14.90 | BLGL |
| ATOM | 423 | CG2 | VAL | 65 | 12.536 | 12.055 | 33.975 | 1.00 | 14.25 | BLGL |
| ATOM | 424 | C | VAL | 65 | 10.847 | 8.668 | 33.414 | 1.00 | 15.70 | BLGL |
| ATOM | 425 | O | VAL | 65 | 9.621 | 8.691 | 33.388 | 1.00 | 16.30 | BLGL |
| ATOM | 426 | N | ARG | 66 | 11.548 | 7.587 | 33.740 | 1.00 | 15.28 | BLGL |
| ATOM | 427 | CA | ARG | 66 | 10.898 | 6.343 | 34.126 | 1.00 | 14.69 | BLGL |
| ATOM | 428 | CB | ARG | 66 | 11.520 | 5.145 | 33.396 | 1.00 | 12.92 | BLGL |
| ATOM | 429 | CG | ARG | 66 | 10.676 | 3.897 | 33.521 | 1.00 | 16.36 | BLGL |
| ATOM | 430 | CD | ARG | 66 | 11.131 | 2.751 | 32.621 | 1.00 | 17.95 | BLGL |
| ATOM | 431 | NE | ARG | 66 | 11.997 | 1.835 | 33.347 | 1.00 | 21.82 | BLGL |
| ATOM | 432 | CZ | ARG | 66 | 11.882 | 0.514 | 33.336 | 1.00 | 20.23 | BLGL |
| ATOM | 433 | NH1 | ARG | 66 | 10.933 | -0.072 | 32.628 | 1.00 | 20.47 | BLGL |
| ATOM | 434 | NH2 | ARG | 66 | 12.720 | -0.218 | 34.050 | 1.00 | 22.65 | BLGL |
| ATOM | 435 | C | ARG | 66 | 11.049 | 6.155 | 35.627 | 1.00 | 15.52 | BLGL |
| ATOM | 436 | O | ARG | 66 | 12.097 | 6.461 | 36.194 | 1.00 | 19.23 | BLGL |
| ATOM | 437 | N | VAL | 67 | 10.003 | 5.663 | 36.277 | 1.00 | 14.45 | BLGL |
| ATOM | 438 | CA | VAL | 67 | 10.065 | 5.437 | 37.709 | 1.00 | 14.29 | BLGL |
| ATOM | 439 | CB | VAL | 67 | 9.387 | 6.591 | 38.500 | 1.00 | 14.34 | BLGL |
| ATOM | 440 | CG1 | VAL | 67 | 8.010 | 6.866 | 37.946 | 1.00 | 15.07 | BLGL |
| ATOM | 441 | CG2 | VAL | 67 | 9.279 | 6.226 | 39.974 | 1.00 | 14.76 | BLGL |
| ATOM | 442 | C | VAL | 67 | 9.380 | 4.134 | 38.050 | 1.00 | 13.80 | BLGL |
| ATOM | 443 | O | VAL | 67 | 8.243 | 3.902 | 37.652 | 1.00 | 16.06 | BLGL |
| ATOM | 444 | N | ARG | 68 | 10.084 | 3.274 | 38.772 | 1.00 | 12.24 | BLGL |
| ATOM | 445 | CA | ARG | 68 | 9.512 | 2.007 | 39.170 | 1.00 | 13.36 | BLGL |
| ATOM | 446 | CB | ARG | 68 | 10.613 | 0.987 | 39.505 | 1.00 | 15.94 | BLGL |
| ATOM | 447 | CG | ARG | 68 | 11.653 | 1.445 | 40.530 | 1.00 | 16.59 | BLGL |
| ATOM | 448 | CD | ARG | 68 | 12.582 | 0.299 | 40.946 | 1.00 | 17.71 | BLGL |
| ATOM | 449 | NE | ARG | 68 | 13.727 | 0.787 | 41.717 | 1.00 | 20.66 | BLGL |
| ATOM | 450 | CZ | ARG | 68 | 14.806 | 1.365 | 41.187 | 1.00 | 19.69 | BLGL |
| ATOM | 451 | NH1 | ARG | 68 | 15.791 | 1.788 | 41.964 | 1.00 | 18.60 | BLGL |
| ATOM | 452 | NH2 | ARG | 68 | 14.912 | 1.502 | 39.876 | 1.00 | 19.53 | BLGL |
| ATOM | 453 | C | ARG | 68 | 8.621 | 2.250 | 40.383 | 1.00 | 16.28 | BLGL |
| ATOM | 454 | O | ARG | 68 | 8.875 | 3.152 | 41.185 | 1.00 | 13.92 | BLGL |
| ATOM | 455 | N | ILE | 69 | 7.567 | 1.449 | 40.506 | 1.00 | 16.59 | BLGL |
| ATOM | 456 | CA | ILE | 69 | 6.649 | 1.582 | 41.619 | 1.00 | 17.08 | BLGL |
| ATOM | 457 | CB | ILE | 69 | 5.331 | 2.254 | 41.176 | 1.00 | 17.80 | BLGL |
| ATOM | 458 | CG2 | ILE | 69 | 4.442 | 2.505 | 42.392 | 1.00 | 16.20 | BLGL |
| ATOM | 459 | CG1 | ILE | 69 | 5.634 | 3.577 | 40.463 | 1.00 | 18.54 | BLGL |
| ATOM | 460 | CD1 | ILE | 69 | 4.420 | 4.258 | 39.861 | 1.00 | 16.60 | BLGL |
| ATOM | 461 | C | ILE | 69 | 6.326 | 0.224 | 42.227 | 1.00 | 19.49 | BLGL |

## Fig. 4 cont.

| | | | | | | | | | | |
|------|-----|-----|-----|----|---------|---------|--------|------|-------|------|
| ATOM | 462 | O | ILE | 69 | 5.851 | -0.684 | 41.537 | 1.00 | 21.07 | BLGL |
| ATOM | 463 | N | TRP | 70 | 6.613 | 0.088 | 43.518 | 1.00 | 19.80 | BLGL |
| ATOM | 464 | CA | TRP | 70 | 6.329 | -1.132 | 44.261 | 1.00 | 20.02 | BLGL |
| ATOM | 465 | CB | TRP | 70 | 7.534 | -1.548 | 45.108 | 1.00 | 20.03 | BLGL |
| ATOM | 466 | CG | TRP | 70 | 8.693 | -2.052 | 44.299 | 1.00 | 20.74 | BLGL |
| ATOM | 467 | CD2 | TRP | 70 | 10.078 | -1.707 | 44.460 | 1.00 | 20.58 | BLGL |
| ATOM | 468 | CE2 | TRP | 70 | 10.807 | -2.445 | 43.496 | 1.00 | 20.35 | BLGL |
| ATOM | 469 | CE3 | TRP | 70 | 10.774 | -0.847 | 45.322 | 1.00 | 19.46 | BLGL |
| ATOM | 470 | CD1 | TRP | 70 | 8.643 | -2.958 | 43.278 | 1.00 | 20.51 | BLGL |
| ATOM | 471 | NE1 | TRP | 70 | 9.906 | -3.198 | 42.791 | 1.00 | 18.08 | BLGL |
| ATOM | 472 | CZ2 | TRP | 70 | 12.200 | -2.350 | 43.372 | 1.00 | 17.40 | BLGL |
| ATOM | 473 | CZ3 | TRP | 70 | 12.162 | -0.752 | 45.197 | 1.00 | 18.53 | BLGL |
| ATOM | 474 | CH2 | TRP | 70 | 12.856 | -1.501 | 44.227 | 1.00 | 17.88 | BLGL |
| ATOM | 475 | C | TRP | 70 | 5.145 | -0.805 | 45.164 | 1.00 | 21.18 | BLGL |
| ATOM | 476 | O | TRP | 70 | 5.010 | 0.328 | 45.626 | 1.00 | 20.39 | BLGL |
| ATOM | 477 | N | ASN | 71 | 4.279 | -1.782 | 45.405 | 1.00 | 21.89 | BLGL |
| ATOM | 478 | CA | ASN | 71 | 3.105 | -1.553 | 46.238 | 1.00 | 23.11 | BLGL |
| ATOM | 479 | CB | ASN | 71 | 2.204 | -2.787 | 46.234 | 1.00 | 21.89 | BLGL |
| ATOM | 480 | CG | ASN | 71 | 1.600 | -3.059 | 44.875 | 1.00 | 24.42 | BLGL |
| ATOM | 481 | OD1 | ASN | 71 | 2.312 | -3.325 | 43.907 | 1.00 | 24.93 | BLGL |
| ATOM | 482 | ND2 | ASN | 71 | 0.277 | -2.986 | 44.792 | 1.00 | 24.52 | BLGL |
| ATOM | 483 | C | ASN | 71 | 3.454 | -1.182 | 47.673 | 1.00 | 23.89 | BLGL |
| ATOM | 484 | O | ASN | 71 | 3.114 | -0.093 | 48.150 | 1.00 | 23.65 | BLGL |
| ATOM | 485 | N | ASP | 72 | 4.139 | -2.094 | 48.356 | 1.00 | 25.19 | BLGL |
| ATOM | 486 | CA | ASP | 72 | 4.531 | -1.888 | 49.747 | 1.00 | 24.90 | BLGL |
| ATOM | 487 | CB | ASP | 72 | 3.576 | -2.642 | 50.669 | 1.00 | 24.77 | BLGL |
| ATOM | 488 | CG | ASP | 72 | 3.706 | -2.214 | 52.105 | 1.00 | 25.24 | BLGL |
| ATOM | 489 | OD1 | ASP | 72 | 3.494 | -3.063 | 52.990 | 1.00 | 26.84 | BLGL |
| ATOM | 490 | OD2 | ASP | 72 | 4.006 | -1.026 | 52.346 | 1.00 | 24.35 | BLGL |
| ATOM | 491 | C | ASP | 72 | 5.953 | -2.384 | 49.997 | 1.00 | 24.58 | BLGL |
| ATOM | 492 | O | ASP | 72 | 6.151 | -3.472 | 50.538 | 1.00 | 25.47 | BLGL |
| ATOM | 493 | N | PRO | 73 | 6.962 | -1.586 | 49.619 | 1.00 | 24.27 | BLGL |
| ATOM | 494 | CD | PRO | 73 | 6.856 | -0.281 | 48.940 | 1.00 | 23.33 | BLGL |
| ATOM | 495 | CA | PRO | 73 | 8.366 | -1.962 | 49.805 | 1.00 | 24.32 | BLGL |
| ATOM | 496 | CB | PRO | 73 | 9.091 | -1.009 | 48.866 | 1.00 | 24.01 | BLGL |
| ATOM | 497 | CG | PRO | 73 | 8.272 | 0.237 | 49.001 | 1.00 | 23.40 | BLGL |
| ATOM | 498 | C | PRO | 73 | 8.863 | -1.840 | 51.248 | 1.00 | 27.14 | BLGL |
| ATOM | 499 | O | PRO | 73 | 9.987 | -1.395 | 51.491 | 1.00 | 28.54 | BLGL |
| ATOM | 500 | N | TYR | 74 | 8.033 | -2.233 | 52.208 | 1.00 | 27.12 | BLGL |
| ATOM | 501 | CA | TYR | 74 | 8.429 | -2.147 | 53.609 | 1.00 | 26.57 | BLGL |
| ATOM | 502 | CB | TYR | 74 | 7.838 | -0.889 | 54.256 | 1.00 | 25.70 | BLGL |
| ATOM | 503 | CG | TYR | 74 | 8.022 | 0.386 | 53.463 | 1.00 | 21.92 | BLGL |
| ATOM | 504 | CD1 | TYR | 74 | 7.148 | 0.721 | 52.427 | 1.00 | 22.26 | BLGL |
| ATOM | 505 | CE1 | TYR | 74 | 7.304 | 1.909 | 51.707 | 1.00 | 21.83 | BLGL |
| ATOM | 506 | CD2 | TYR | 74 | 9.057 | 1.265 | 53.758 | 1.00 | 18.92 | BLGL |
| ATOM | 507 | CE2 | TYR | 74 | 9.223 | 2.448 | 53.049 | 1.00 | 19.47 | BLGL |
| ATOM | 508 | CZ | TYR | 74 | 8.345 | 2.766 | 52.026 | 1.00 | 21.06 | BLGL |
| ATOM | 509 | OH | TYR | 74 | 8.503 | 3.939 | 51.323 | 1.00 | 21.16 | BLGL |
| ATOM | 510 | C | TYR | 74 | 7.970 | -3.371 | 54.395 | 1.00 | 26.69 | BLGL |
| ATOM | 511 | O | TYR | 74 | 7.119 | -4.131 | 53.928 | 1.00 | 26.70 | BLGL |
| ATOM | 512 | N | ASP | 75 | 8.547 | -3.568 | 55.579 | 1.00 | 25.47 | BLGL |
| ATOM | 513 | CA | ASP | 75 | 8.151 | -4.687 | 56.422 | 1.00 | 25.66 | BLGL |
| ATOM | 514 | CB | ASP | 75 | 9.348 | -5.260 | 57.201 | 1.00 | 26.96 | BLGL |
| ATOM | 515 | CG | ASP | 75 | 9.948 | -4.282 | 58.207 | 1.00 | 26.69 | BLGL |
| ATOM | 516 | OD1 | ASP | 75 | 10.931 | -4.668 | 58.867 | 1.00 | 25.84 | BLGL |
| ATOM | 517 | OD2 | ASP | 75 | 9.455 | -3.146 | 58.350 | 1.00 | 28.52 | BLGL |
| ATOM | 518 | C | ASP | 75 | 7.060 | -4.208 | 57.367 | 1.00 | 26.20 | BLGL |
| ATOM | 519 | O | ASP | 75 | 6.634 | -3.063 | 57.286 | 1.00 | 27.42 | BLGL |
| ATOM | 520 | N | ALA | 76 | 6.602 | -5.078 | 58.255 | 1.00 | 27.05 | BLGL |
| ATOM | 521 | CA | ALA | 76 | 5.535 | -4.722 | 59.184 | 1.00 | 28.91 | BLGL |
| ATOM | 522 | CB | ALA | 76 | 5.304 | -5.869 | 60.153 | 1.00 | 29.44 | BLGL |
| ATOM | 523 | C | ALA | 76 | 5.793 | -3.438 | 59.964 | 1.00 | 29.89 | BLGL |
| ATOM | 524 | O | ALA | 76 | 4.873 | -2.666 | 60.241 | 1.00 | 31.61 | BLGL |
| ATOM | 525 | N | ASN | 77 | 7.051 | -3.213 | 60.307 | 1.00 | 29.94 | BLGL |
| ATOM | 526 | CA | ASN | 77 | 7.445 | -2.059 | 61.091 | 1.00 | 30.08 | BLGL |
| ATOM | 527 | CB | ASN | 77 | 8.619 | -2.460 | 61.970 | 1.00 | 30.88 | BLGL |

# Fig. 4 cont.

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 528 | CG | ASN | 77 | 8.337 | -3.728 | 62.740 | 1.00 | 31.46 | BLGL |
| ATOM | 529 | OD1 | ASN | 77 | 9.085 | -4.700 | 62.659 | 1.00 | 35.40 | BLGL |
| ATOM | 530 | ND2 | ASN | 77 | 7.241 | -3.729 | 63.485 | 1.00 | 29.08 | BLGL |
| ATOM | 531 | C | ASN | 77 | 7.768 | -0.802 | 60.294 | 1.00 | 30.14 | BLGL |
| ATOM | 532 | O | ASN | 77 | 8.048 | 0.249 | 60.874 | 1.00 | 31.47 | BLGL |
| ATOM | 533 | N | GLY | 78 | 7.742 | -0.906 | 58.971 | 1.00 | 29.60 | BLGL |
| ATOM | 534 | CA | GLY | 78 | 7.998 | 0.260 | 58.146 | 1.00 | 30.47 | BLGL |
| ATOM | 535 | C | GLY | 78 | 9.422 | 0.434 | 57.665 | 1.00 | 30.69 | BLGL |
| ATOM | 536 | O | GLY | 78 | 9.803 | 1.524 | 57.243 | 1.00 | 31.23 | BLGL |
| ATOM | 537 | N | ASN | 79 | 10.212 | -0.631 | 57.735 | 1.00 | 30.64 | BLGL |
| ATOM | 538 | CA | ASN | 79 | 11.599 | -0.586 | 57.285 | 1.00 | 31.66 | BLGL |
| ATOM | 539 | CB | ASN | 79 | 12.437 | -1.618 | 58.043 | 1.00 | 32.77 | BLGL |
| ATOM | 540 | CG | ASN | 79 | 12.478 | -1.356 | 59.539 | 1.00 | 32.28 | BLGL |
| ATOM | 541 | OD1 | ASN | 79 | 12.875 | -0.277 | 59.981 | 1.00 | 31.97 | BLGL |
| ATOM | 542 | ND2 | ASN | 79 | 12.074 | -2.346 | 60.325 | 1.00 | 29.86 | BLGL |
| ATOM | 543 | C | ASN | 79 | 11.652 | -0.888 | 55.788 | 1.00 | 31.40 | BLGL |
| ATOM | 544 | O | ASN | 79 | 11.253 | -1.971 | 55.352 | 1.00 | 31.55 | BLGL |
| ATOM | 545 | N | GLY | 80 | 12.146 | 0.072 | 55.013 | 1.00 | 30.48 | BLGL |
| ATOM | 546 | CA | GLY | 80 | 12.224 | -0.092 | 53.573 | 1.00 | 28.01 | BLGL |
| ATOM | 547 | C | GLY | 80 | 13.066 | -1.265 | 53.132 | 1.00 | 26.92 | BLGL |
| ATOM | 548 | O | GLY | 80 | 14.104 | -1.544 | 53.737 | 1.00 | 28.09 | BLGL |
| ATOM | 549 | N | TYR | 81 | 12.611 | -1.958 | 52.089 | 1.00 | 25.24 | BLGL |
| ATOM | 550 | CA | TYR | 81 | 13.330 | -3.110 | 51.539 | 1.00 | 24.70 | BLGL |
| ATOM | 551 | CB | TYR | 81 | 12.446 | -3.891 | 50.559 | 1.00 | 26.19 | BLGL |
| ATOM | 552 | CG | TYR | 81 | 11.309 | -4.704 | 51.155 | 1.00 | 28.51 | BLGL |
| ATOM | 553 | CD1 | TYR | 81 | 10.337 | -5.264 | 50.324 | 1.00 | 30.98 | BLGL |
| ATOM | 554 | CE1 | TYR | 81 | 9.285 | -6.014 | 50.836 | 1.00 | 33.39 | BLGL |
| ATOM | 555 | CD2 | TYR | 81 | 11.202 | -4.919 | 52.525 | 1.00 | 27.25 | BLGL |
| ATOM | 556 | CE2 | TYR | 81 | 10.151 | -5.673 | 53.053 | 1.00 | 30.71 | BLGL |
| ATOM | 557 | CZ | TYR | 81 | 9.191 | -6.218 | 52.201 | 1.00 | 32.59 | BLGL |
| ATOM | 558 | OH | TYR | 81 | 8.134 | -6.955 | 52.701 | 1.00 | 29.32 | BLGL |
| ATOM | 559 | C | TYR | 81 | 14.581 | -2.643 | 50.791 | 1.00 | 23.17 | BLGL |
| ATOM | 560 | O | TYR | 81 | 15.424 | -3.449 | 50.411 | 1.00 | 22.30 | BLGL |
| ATOM | 561 | N | GLY | 82 | 14.692 | -1.337 | 50.575 | 1.00 | 22.25 | BLGL |
| ATOM | 562 | CA | GLY | 82 | 15.840 | -0.812 | 49.863 | 1.00 | 22.06 | BLGL |
| ATOM | 563 | C | GLY | 82 | 15.544 | -0.631 | 48.388 | 1.00 | 23.07 | BLGL |
| ATOM | 564 | O | GLY | 82 | 14.392 | -0.466 | 47.994 | 1.00 | 22.83 | BLGL |
| ATOM | 565 | N | GLY | 83 | 16.582 | -0.660 | 47.561 | 1.00 | 23.84 | BLGL |
| ATOM | 566 | CA | GLY | 83 | 16.384 | -0.485 | 46.133 | 1.00 | 23.31 | BLGL |
| ATOM | 567 | C | GLY | 83 | 15.731 | 0.843 | 45.796 | 1.00 | 23.19 | BLGL |
| ATOM | 568 | O | GLY | 83 | 15.219 | 1.024 | 44.693 | 1.00 | 23.86 | BLGL |
| ATOM | 569 | N | GLY | 84 | 15.740 | 1.772 | 46.748 | 1.00 | 22.55 | BLGL |
| ATOM | 570 | CA | GLY | 84 | 15.142 | 3.075 | 46.514 | 1.00 | 18.60 | BLGL |
| ATOM | 571 | C | GLY | 84 | 13.832 | 3.262 | 47.243 | 1.00 | 18.25 | BLGL |
| ATOM | 572 | O | GLY | 84 | 13.282 | 4.354 | 47.254 | 1.00 | 19.59 | BLGL |
| ATOM | 573 | N | ASN | 85 | 13.339 | 2.199 | 47.867 | 1.00 | 18.82 | BLGL |
| ATOM | 574 | CA | ASN | 85 | 12.070 | 2.246 | 48.591 | 1.00 | 22.71 | BLGL |
| ATOM | 575 | CB | ASN | 85 | 12.217 | 3.011 | 49.914 | 1.00 | 22.20 | BLGL |
| ATOM | 576 | CG | ASN | 85 | 13.143 | 2.319 | 50.902 | 1.00 | 24.42 | BLGL |
| ATOM | 577 | OD1 | ASN | 85 | 13.320 | 1.102 | 50.869 | 1.00 | 25.77 | BLGL |
| ATOM | 578 | ND2 | ASN | 85 | 13.721 | 3.098 | 51.806 | 1.00 | 25.80 | BLGL |
| ATOM | 579 | C | ASN | 85 | 11.004 | 2.929 | 47.729 | 1.00 | 23.49 | BLGL |
| ATOM | 580 | O | ASN | 85 | 10.235 | 3.761 | 48.214 | 1.00 | 23.21 | BLGL |
| ATOM | 581 | N | ASN | 86 | 10.950 | 2.566 | 46.452 | 1.00 | 23.70 | BLGL |
| ATOM | 582 | CA | ASN | 86 | 10.001 | 3.196 | 45.546 | 1.00 | 24.44 | BLGL |
| ATOM | 583 | CB | ASN | 86 | 10.447 | 3.008 | 44.106 | 1.00 | 21.35 | BLGL |
| ATOM | 584 | CG | ASN | 86 | 11.781 | 3.627 | 43.847 | 1.00 | 21.48 | BLGL |
| ATOM | 585 | OD1 | ASN | 86 | 12.811 | 2.972 | 43.976 | 1.00 | 22.65 | BLGL |
| ATOM | 586 | ND2 | ASN | 86 | 11.781 | 4.908 | 43.500 | 1.00 | 20.47 | BLGL |
| ATOM | 587 | C | ASN | 86 | 8.546 | 2.785 | 45.679 | 1.00 | 25.13 | BLGL |
| ATOM | 588 | O | ASN | 86 | 8.159 | 1.666 | 45.357 | 1.00 | 23.77 | BLGL |
| ATOM | 589 | N | ASP | 87 | 7.742 | 3.723 | 46.155 | 1.00 | 25.52 | BLGL |
| ATOM | 590 | CA | ASP | 87 | 6.323 | 3.500 | 46.323 | 1.00 | 26.02 | BLGL |
| ATOM | 591 | CB | ASP | 87 | 5.954 | 3.547 | 47.803 | 1.00 | 25.67 | BLGL |
| ATOM | 592 | CG | ASP | 87 | 6.584 | 4.724 | 48.524 | 1.00 | 30.07 | BLGL |
| ATOM | 593 | OD1 | ASP | 87 | 6.994 | 5.705 | 47.851 | 1.00 | 29.90 | BLGL |

# Fig. 4 cont.

| ATOM | 594 | OD2 | ASP | 87 | 6.656 | 4.668 | 49.771 | 1.00 | 31.21 | BLGL |
|------|-----|-----|-----|-----|-------|-------|--------|------|-------|------|
| ATOM | 595 | C | ASP | 87 | 5.625 | 4.613 | 45.566 | 1.00 | 25.13 | BLGL |
| ATOM | 596 | O | ASP | 87 | 6.276 | 5.396 | 44.877 | 1.00 | 25.07 | BLGL |
| ATOM | 597 | N | LEU | 88 | 4.307 | 4.693 | 45.694 | 1.00 | 25.05 | BLGL |
| ATOM | 598 | CA | LEU | 88 | 3.566 | 5.732 | 44.996 | 1.00 | 27.31 | BLGL |
| ATOM | 599 | CB | LEU | 88 | 2.059 | 5.528 | 45.183 | 1.00 | 25.49 | BLGL |
| ATOM | 600 | CG | LEU | 88 | 1.163 | 6.603 | 44.564 | 1.00 | 23.47 | BLGL |
| ATOM | 601 | CD1 | LEU | 88 | 1.378 | 6.668 | 43.059 | 1.00 | 23.31 | BLGL |
| ATOM | 602 | CD2 | LEU | 88 | −0.283 | 6.294 | 44.880 | 1.00 | 23.48 | BLGL |
| ATOM | 603 | C | LEU | 88 | 3.956 | 7.146 | 45.440 | 1.00 | 28.05 | BLGL |
| ATOM | 604 | O | LEU | 88 | 3.942 | 8.072 | 44.633 | 1.00 | 28.88 | BLGL |
| ATOM | 605 | N | GLU | 89 | 4.310 | 7.312 | 46.713 | 1.00 | 28.47 | BLGL |
| ATOM | 606 | CA | GLU | 89 | 4.679 | 8.627 | 47.223 | 1.00 | 31.19 | BLGL |
| ATOM | 607 | CB | GLU | 89 | 4.884 | 8.596 | 48.743 | 1.00 | 38.35 | BLGL |
| ATOM | 608 | CG | GLU | 89 | 4.732 | 7.224 | 49.404 | 1.00 | 49.47 | BLGL |
| ATOM | 609 | CD | GLU | 89 | 3.309 | 6.673 | 49.355 | 1.00 | 54.88 | BLGL |
| ATOM | 610 | OE1 | GLU | 89 | 3.095 | 5.617 | 48.709 | 1.00 | 55.88 | BLGL |
| ATOM | 611 | OE2 | GLU | 89 | 2.413 | 7.297 | 49.968 | 1.00 | 58.86 | BLGL |
| ATOM | 612 | C | GLU | 89 | 5.931 | 9.157 | 46.547 | 1.00 | 28.83 | BLGL |
| ATOM | 613 | O | GLU | 89 | 5.958 | 10.293 | 46.083 | 1.00 | 29.30 | BLGL |
| ATOM | 614 | N | LYS | 90 | 6.970 | 8.337 | 46.486 | 1.00 | 27.00 | BLGL |
| ATOM | 615 | CA | LYS | 90 | 8.202 | 8.758 | 45.833 | 1.00 | 25.31 | BLGL |
| ATOM | 616 | CB | LYS | 90 | 9.308 | 7.731 | 46.074 | 1.00 | 24.21 | BLGL |
| ATOM | 617 | CG | LYS | 90 | 9.730 | 7.618 | 47.526 | 1.00 | 23.42 | BLGL |
| ATOM | 618 | CD | LYS | 90 | 11.003 | 6.815 | 47.664 | 1.00 | 23.39 | BLGL |
| ATOM | 619 | CE | LYS | 90 | 11.521 | 6.845 | 49.092 | 1.00 | 22.77 | BLGL |
| ATOM | 620 | NZ | LYS | 90 | 10.589 | 6.181 | 50.039 | 1.00 | 24.27 | BLGL |
| ATOM | 621 | C | LYS | 90 | 7.966 | 8.940 | 44.333 | 1.00 | 24.86 | BLGL |
| ATOM | 622 | O | LYS | 90 | 8.604 | 9.779 | 43.696 | 1.00 | 23.88 | BLGL |
| ATOM | 623 | N | ALA | 91 | 7.043 | 8.157 | 43.776 | 1.00 | 22.89 | BLGL |
| ATOM | 624 | CA | ALA | 91 | 6.727 | 8.252 | 42.362 | 1.00 | 23.29 | BLGL |
| ATOM | 625 | CB | ALA | 91 | 5.709 | 7.175 | 41.972 | 1.00 | 21.21 | BLGL |
| ATOM | 626 | C | ALA | 91 | 6.172 | 9.644 | 42.060 | 1.00 | 23.82 | BLGL |
| ATOM | 627 | O | ALA | 91 | 6.501 | 10.244 | 41.042 | 1.00 | 24.10 | BLGL |
| ATOM | 628 | N | ILE | 92 | 5.335 | 10.154 | 42.956 | 1.00 | 24.44 | BLGL |
| ATOM | 629 | CA | ILE | 92 | 4.743 | 11.471 | 42.782 | 1.00 | 25.65 | BLGL |
| ATOM | 630 | CB | ILE | 92 | 3.549 | 11.651 | 43.748 | 1.00 | 26.69 | BLGL |
| ATOM | 631 | CG2 | ILE | 92 | 2.943 | 13.041 | 43.600 | 1.00 | 25.04 | BLGL |
| ATOM | 632 | CG1 | ILE | 92 | 2.484 | 10.602 | 43.418 | 1.00 | 27.42 | BLGL |
| ATOM | 633 | CD1 | ILE | 92 | 1.341 | 10.553 | 44.385 | 1.00 | 25.99 | BLGL |
| ATOM | 634 | C | ILE | 92 | 5.794 | 12.568 | 42.992 | 1.00 | 25.95 | BLGL |
| ATOM | 635 | O | ILE | 92 | 5.800 | 13.575 | 42.286 | 1.00 | 26.66 | BLGL |
| ATOM | 636 | N | GLN | 93 | 6.687 | 12.367 | 43.956 | 1.00 | 25.21 | BLGL |
| ATOM | 637 | CA | GLN | 93 | 7.746 | 13.332 | 44.206 | 1.00 | 25.19 | BLGL |
| ATOM | 638 | CB | GLN | 93 | 8.623 | 12.886 | 45.369 | 1.00 | 27.76 | BLGL |
| ATOM | 639 | CG | GLN | 93 | 8.285 | 13.505 | 46.705 | 1.00 | 33.90 | BLGL |
| ATOM | 640 | CD | GLN | 93 | 9.215 | 13.020 | 47.818 | 1.00 | 38.24 | BLGL |
| ATOM | 641 | OE1 | GLN | 93 | 9.088 | 11.890 | 48.303 | 1.00 | 35.85 | BLGL |
| ATOM | 642 | NE2 | GLN | 93 | 10.165 | 13.873 | 48.216 | 1.00 | 40.86 | BLGL |
| ATOM | 643 | C | GLN | 93 | 8.595 | 13.427 | 42.949 | 1.00 | 24.82 | BLGL |
| ATOM | 644 | O | GLN | 93 | 8.870 | 14.514 | 42.454 | 1.00 | 27.29 | BLGL |
| ATOM | 645 | N | ILE | 94 | 9.008 | 12.276 | 42.434 | 1.00 | 23.84 | BLGL |
| ATOM | 646 | CA | ILE | 94 | 9.818 | 12.225 | 41.223 | 1.00 | 21.73 | BLGL |
| ATOM | 647 | CB | ILE | 94 | 10.263 | 10.772 | 40.929 | 1.00 | 20.65 | BLGL |
| ATOM | 648 | CG2 | ILE | 94 | 10.936 | 10.687 | 39.568 | 1.00 | 19.77 | BLGL |
| ATOM | 649 | CG1 | ILE | 94 | 11.202 | 10.293 | 42.043 | 1.00 | 18.55 | BLGL |
| ATOM | 650 | CD1 | ILE | 94 | 11.644 | 8.866 | 41.914 | 1.00 | 12.93 | BLGL |
| ATOM | 651 | C | ILE | 94 | 9.027 | 12.770 | 40.038 | 1.00 | 21.61 | BLGL |
| ATOM | 652 | O | ILE | 94 | 9.545 | 13.553 | 39.232 | 1.00 | 19.49 | BLGL |
| ATOM | 653 | N | GLY | 95 | 7.764 | 12.362 | 39.955 | 1.00 | 22.02 | BLGL |
| ATOM | 654 | CA | GLY | 95 | 6.897 | 12.798 | 38.876 | 1.00 | 23.64 | BLGL |
| ATOM | 655 | C | GLY | 95 | 6.787 | 14.302 | 38.771 | 1.00 | 24.52 | BLGL |
| ATOM | 656 | O | GLY | 95 | 6.932 | 14.870 | 37.683 | 1.00 | 24.81 | BLGL |
| ATOM | 657 | N | LYS | 96 | 6.526 | 14.947 | 39.907 | 1.00 | 26.80 | BLGL |
| ATOM | 658 | CA | LYS | 96 | 6.401 | 16.403 | 39.971 | 1.00 | 26.56 | BLGL |
| ATOM | 659 | CB | LYS | 96 | 6.095 | 16.844 | 41.401 | 1.00 | 26.83 | BLGL |

**Fig. 4 cont.**

| ATOM | 660 | CG | LYS | 96 | 4.653 | 16.630 | 41.818 | 1.00 | 30.58 | BLGL |
|------|-----|-----|-----|-----|--------|--------|--------|------|-------|------|
| ATOM | 661 | CD | LYS | 96 | 4.413 | 17.224 | 43.192 | 1.00 | 34.86 | BLGL |
| ATOM | 662 | CE | LYS | 96 | 2.939 | 17.256 | 43.541 | 1.00 | 38.91 | BLGL |
| ATOM | 663 | NZ | LYS | 96 | 2.712 | 17.810 | 44.909 | 1.00 | 42.19 | BLGL |
| ATOM | 664 | C | LYS | 96 | 7.663 | 17.106 | 39.474 | 1.00 | 26.13 | BLGL |
| ATOM | 665 | O | LYS | 96 | 7.592 | 18.041 | 38.676 | 1.00 | 25.77 | BLGL |
| ATOM | 666 | N | ARG | 97 | 8.818 | 16.649 | 39.946 | 1.00 | 26.45 | BLGL |
| ATOM | 667 | CA | ARG | 97 | 10.089 | 17.232 | 39.533 | 1.00 | 25.62 | BLGL |
| ATOM | 668 | CB | ARG | 97 | 11.229 | 16.598 | 40.335 | 1.00 | 26.14 | BLGL |
| ATOM | 669 | CG | ARG | 97 | 11.105 | 16.909 | 41.824 | 1.00 | 28.26 | BLGL |
| ATOM | 670 | CD | ARG | 97 | 12.157 | 16.228 | 42.687 | 1.00 | 28.70 | BLGL |
| ATOM | 671 | NE | ARG | 97 | 13.514 | 16.674 | 42.385 | 1.00 | 30.96 | BLGL |
| ATOM | 672 | CZ | ARG | 97 | 14.593 | 16.211 | 43.007 | 1.00 | 29.36 | BLGL |
| ATOM | 673 | NH1 | ARG | 97 | 14.460 | 15.297 | 43.959 | 1.00 | 26.96 | BLGL |
| ATOM | 674 | NH2 | ARG | 97 | 15.799 | 16.650 | 42.671 | 1.00 | 26.20 | BLGL |
| ATOM | 675 | C | ARG | 97 | 10.310 | 17.060 | 38.032 | 1.00 | 24.94 | BLGL |
| ATOM | 676 | O | ARG | 97 | 10.778 | 17.973 | 37.354 | 1.00 | 24.07 | BLGL |
| ATOM | 677 | N | ALA | 98 | 9.959 | 15.890 | 37.510 | 1.00 | 24.88 | BLGL |
| ATOM | 678 | CA | ALA | 98 | 10.104 | 15.626 | 36.084 | 1.00 | 24.73 | BLGL |
| ATOM | 679 | CB | ALA | 98 | 9.673 | 14.198 | 35.771 | 1.00 | 26.89 | BLGL |
| ATOM | 680 | C | ALA | 98 | 9.265 | 16.620 | 35.277 | 1.00 | 24.32 | BLGL |
| ATOM | 681 | O | ALA | 98 | 9.715 | 17.145 | 34.256 | 1.00 | 21.35 | BLGL |
| ATOM | 682 | N | ASN | 99 | 8.041 | 16.875 | 35.727 | 1.00 | 25.11 | BLGL |
| ATOM | 683 | CA | ASN | 99 | 7.196 | 17.830 | 35.019 | 1.00 | 27.26 | BLGL |
| ATOM | 684 | CB | ASN | 99 | 5.802 | 17.871 | 35.601 | 1.00 | 29.92 | BLGL |
| ATOM | 685 | CG | ASN | 99 | 5.039 | 16.631 | 35.330 | 1.00 | 36.77 | BLGL |
| ATOM | 686 | OD1 | ASN | 99 | 3.817 | 16.649 | 35.364 | 1.00 | 43.97 | BLGL |
| ATOM | 687 | ND2 | ASN | 99 | 5.743 | 15.529 | 35.063 | 1.00 | 38.67 | BLGL |
| ATOM | 688 | C | ASN | 99 | 7.766 | 19.229 | 35.096 | 1.00 | 26.84 | BLGL |
| ATOM | 689 | O | ASN | 99 | 7.850 | 19.919 | 34.090 | 1.00 | 29.38 | BLGL |
| ATOM | 690 | N | ALA | 100 | 8.143 | 19.652 | 36.298 | 1.00 | 23.90 | BLGL |
| ATOM | 691 | CA | ALA | 100 | 8.689 | 20.982 | 36.481 | 1.00 | 23.21 | BLGL |
| ATOM | 692 | CB | ALA | 100 | 9.214 | 21.137 | 37.894 | 1.00 | 20.39 | BLGL |
| ATOM | 693 | C | ALA | 100 | 9.800 | 21.244 | 35.470 | 1.00 | 25.29 | BLGL |
| ATOM | 694 | O | ALA | 100 | 10.088 | 22.394 | 35.141 | 1.00 | 26.23 | BLGL |
| ATOM | 695 | N | ASN | 101 | 10.409 | 20.174 | 34.963 | 1.00 | 25.14 | BLGL |
| ATOM | 696 | CA | ASN | 101 | 11.492 | 20.307 | 33.998 | 1.00 | 25.17 | BLGL |
| ATOM | 697 | CB | ASN | 101 | 12.696 | 19.515 | 34.483 | 1.00 | 24.95 | BLGL |
| ATOM | 698 | CG | ASN | 101 | 13.280 | 20.091 | 35.747 | 1.00 | 25.85 | BLGL |
| ATOM | 699 | OD1 | ASN | 101 | 13.914 | 21.145 | 35.719 | 1.00 | 29.40 | BLGL |
| ATOM | 700 | ND2 | ASN | 101 | 13.054 | 19.422 | 36.868 | 1.00 | 24.97 | BLGL |
| ATOM | 701 | C | ASN | 101 | 11.118 | 19.898 | 32.582 | 1.00 | 25.90 | BLGL |
| ATOM | 702 | O | ASN | 101 | 11.978 | 19.563 | 31.772 | 1.00 | 27.14 | BLGL |
| ATOM | 703 | N | GLY | 102 | 9.824 | 19.932 | 32.290 | 1.00 | 25.80 | BLGL |
| ATOM | 704 | CA | GLY | 102 | 9.345 | 19.598 | 30.962 | 1.00 | 24.78 | BLGL |
| ATOM | 705 | C | GLY | 102 | 9.671 | 18.215 | 30.447 | 1.00 | 25.83 | BLGL |
| ATOM | 706 | O | GLY | 102 | 10.048 | 18.061 | 29.289 | 1.00 | 27.54 | BLGL |
| ATOM | 707 | N | MET | 103 | 9.525 | 17.205 | 31.297 | 1.00 | 26.80 | BLGL |
| ATOM | 708 | CA | MET | 103 | 9.793 | 15.827 | 30.899 | 1.00 | 26.04 | BLGL |
| ATOM | 709 | CB | MET | 103 | 11.006 | 15.283 | 31.662 | 1.00 | 26.48 | BLGL |
| ATOM | 710 | CG | MET | 103 | 12.265 | 16.110 | 31.451 | 1.00 | 29.27 | BLGL |
| ATOM | 711 | SD | MET | 103 | 13.767 | 15.380 | 32.124 | 1.00 | 31.74 | BLGL |
| ATOM | 712 | CE | MET | 103 | 13.716 | 16.017 | 33.804 | 1.00 | 31.73 | BLGL |
| ATOM | 713 | C | MET | 103 | 8.559 | 14.978 | 31.191 | 1.00 | 25.31 | BLGL |
| ATOM | 714 | O | MET | 103 | 7.892 | 15.179 | 32.206 | 1.00 | 24.54 | BLGL |
| ATOM | 715 | N | LYS | 104 | 8.243 | 14.044 | 30.294 | 1.00 | 24.62 | BLGL |
| ATOM | 716 | CA | LYS | 104 | 7.082 | 13.174 | 30.484 | 1.00 | 24.42 | BLGL |
| ATOM | 717 | CB | LYS | 104 | 6.668 | 12.527 | 29.167 | 1.00 | 28.12 | BLGL |
| ATOM | 718 | CG | LYS | 104 | 6.265 | 13.483 | 28.062 | 1.00 | 32.81 | BLGL |
| ATOM | 719 | CD | LYS | 104 | 4.800 | 13.820 | 28.149 | 1.00 | 35.64 | BLGL |
| ATOM | 720 | CE | LYS | 104 | 4.294 | 14.402 | 26.843 | 1.00 | 37.37 | BLGL |
| ATOM | 721 | NZ | LYS | 104 | 2.807 | 14.485 | 26.870 | 1.00 | 40.79 | BLGL |
| ATOM | 722 | C | LYS | 104 | 7.452 | 12.075 | 31.466 | 1.00 | 22.98 | BLGL |
| ATOM | 723 | O | LYS | 104 | 8.632 | 11.840 | 31.720 | 1.00 | 23.51 | BLGL |
| ATOM | 724 | N | LEU | 105 | 6.450 | 11.398 | 32.014 | 1.00 | 21.49 | BLGL |
| ATOM | 725 | CA | LEU | 105 | 6.705 | 10.313 | 32.955 | 1.00 | 19.77 | BLGL |

**Fig. 4 cont.**

| ATOM | 726 | CB | LEU | 105 | 5.975 | 10.559 | 34.279 | 1.00 | 18.76 | BLGL |
|------|-----|------|-----|-----|--------|---------|--------|------|-------|------|
| ATOM | 727 | CG | LEU | 105 | 6.334 | 9.548 | 35.381 | 1.00 | 19.18 | BLGL |
| ATOM | 728 | CD1 | LEU | 105 | 7.586 | 10.007 | 36.100 | 1.00 | 16.56 | BLGL |
| ATOM | 729 | CD2 | LEU | 105 | 5.195 | 9.412 | 36.364 | 1.00 | 21.13 | BLGL |
| ATOM | 730 | C | LEU | 105 | 6.280 | 8.941 | 32.418 | 1.00 | 19.86 | BLGL |
| ATOM | 731 | O | LEU | 105 | 5.285 | 8.812 | 31.701 | 1.00 | 16.96 | BLGL |
| ATOM | 732 | N | LEU | 106 | 7.059 | 7.920 | 32.758 | 1.00 | 19.88 | BLGL |
| ATOM | 733 | CA | LEU | 106 | 6.738 | 6.551 | 32.381 | 1.00 | 19.92 | BLGL |
| ATOM | 734 | CB | LEU | 106 | 7.889 | 5.878 | 31.637 | 1.00 | 17.61 | BLGL |
| ATOM | 735 | CG | LEU | 106 | 7.550 | 4.607 | 30.838 | 1.00 | 21.29 | BLGL |
| ATOM | 736 | CD1 | LEU | 106 | 8.845 | 3.872 | 30.511 | 1.00 | 18.25 | BLGL |
| ATOM | 737 | CD2 | LEU | 106 | 6.627 | 3.689 | 31.604 | 1.00 | 17.96 | BLGL |
| ATOM | 738 | C | LEU | 106 | 6.567 | 5.877 | 33.730 | 1.00 | 19.81 | BLGL |
| ATOM | 739 | O | LEU | 106 | 7.546 | 5.660 | 34.437 | 1.00 | 19.58 | BLGL |
| ATOM | 740 | N | ALA | 107 | 5.327 | 5.581 | 34.102 | 1.00 | 20.44 | BLGL |
| ATOM | 741 | CA | ALA | 107 | 5.052 | 4.922 | 35.373 | 1.00 | 20.99 | BLGL |
| ATOM | 742 | CB | ALA | 107 | 3.634 | 5.240 | 35.826 | 1.00 | 21.52 | BLGL |
| ATOM | 743 | C | ALA | 107 | 5.224 | 3.418 | 35.177 | 1.00 | 21.97 | BLGL |
| ATOM | 744 | O | ALA | 107 | 4.493 | 2.796 | 34.406 | 1.00 | 23.04 | BLGL |
| ATOM | 745 | N | ASP | 108 | 6.192 | 2.828 | 35.867 | 1.00 | 21.22 | BLGL |
| ATOM | 746 | CA | ASP | 108 | 6.438 | 1.400 | 35.726 | 1.00 | 20.00 | BLGL |
| ATOM | 747 | CB | ASP | 108 | 7.932 | 1.175 | 35.463 | 1.00 | 17.66 | BLGL |
| ATOM | 748 | CG | ASP | 108 | 8.327 | -0.289 | 35.455 | 1.00 | 17.79 | BLGL |
| ATOM | 749 | OD1 | ASP | 108 | 7.448 | -1.173 | 35.519 | 1.00 | 16.92 | BLGL |
| ATOM | 750 | OD2 | ASP | 108 | 9.542 | -0.562 | 35.385 | 1.00 | 18.27 | BLGL |
| ATOM | 751 | C | ASP | 108 | 5.966 | 0.625 | 36.953 | 1.00 | 21.24 | BLGL |
| ATOM | 752 | O | ASP | 108 | 6.635 | 0.614 | 37.984 | 1.00 | 25.51 | BLGL |
| ATOM | 753 | N | PHE | 109 | 4.801 | -0.010 | 36.840 | 1.00 | 19.98 | BLGL |
| ATOM | 754 | CA | PHE | 109 | 4.256 | -0.792 | 37.939 | 1.00 | 20.05 | BLGL |
| ATOM | 755 | CB | PHE | 109 | 2.739 | -0.903 | 37.850 | 1.00 | 20.06 | BLGL |
| ATOM | 756 | CG | PHE | 109 | 2.033 | 0.386 | 38.066 | 1.00 | 21.36 | BLGL |
| ATOM | 757 | CD1 | PHE | 109 | 1.751 | 1.225 | 36.995 | 1.00 | 21.28 | BLGL |
| ATOM | 758 | CD2 | PHE | 109 | 1.665 | 0.777 | 39.349 | 1.00 | 21.79 | BLGL |
| ATOM | 759 | CE1 | PHE | 109 | 1.110 | 2.442 | 37.194 | 1.00 | 24.40 | BLGL |
| ATOM | 760 | CE2 | PHE | 109 | 1.026 | 1.989 | 39.564 | 1.00 | 23.03 | BLGL |
| ATOM | 761 | CZ | PHE | 109 | 0.745 | 2.828 | 38.482 | 1.00 | 23.74 | BLGL |
| ATOM | 762 | C | PHE | 109 | 4.822 | -2.190 | 37.949 | 1.00 | 19.77 | BLGL |
| ATOM | 763 | O | PHE | 109 | 4.680 | -2.932 | 36.978 | 1.00 | 18.81 | BLGL |
| ATOM | 764 | N | HIS | 110 | 5.464 | -2.547 | 39.054 | 1.00 | 19.76 | BLGL |
| ATOM | 765 | CA | HIS | 110 | 6.023 | -3.875 | 39.188 | 1.00 | 20.72 | BLGL |
| ATOM | 766 | CB | HIS | 110 | 7.207 | -3.876 | 40.157 | 1.00 | 20.31 | BLGL |
| ATOM | 767 | CG | HIS | 110 | 8.497 | -3.439 | 39.540 | 1.00 | 20.23 | BLGL |
| ATOM | 768 | CD2 | HIS | 110 | 8.779 | -2.456 | 38.653 | 1.00 | 19.83 | BLGL |
| ATOM | 769 | ND1 | HIS | 110 | 9.703 | -4.034 | 39.845 | 1.00 | 21.63 | BLGL |
| ATOM | 770 | CE1 | HIS | 110 | 10.671 | -3.437 | 39.174 | 1.00 | 20.13 | BLGL |
| ATOM | 771 | NE2 | HIS | 110 | 10.137 | -2.475 | 38.442 | 1.00 | 20.13 | BLGL |
| ATOM | 772 | C | HIS | 110 | 4.948 | -4.823 | 39.695 | 1.00 | 20.55 | BLGL |
| ATOM | 773 | O | HIS | 110 | 5.056 | -6.036 | 39.536 | 1.00 | 20.58 | BLGL |
| ATOM | 774 | N | TYR | 111 | 3.900 | -4.267 | 40.291 | 1.00 | 21.08 | BLGL |
| ATOM | 775 | CA | TYR | 111 | 2.827 | -5.093 | 40.830 | 1.00 | 23.38 | BLGL |
| ATOM | 776 | CB | TYR | 111 | 2.039 | -5.759 | 39.695 | 1.00 | 22.62 | BLGL |
| ATOM | 777 | CG | TYR | 111 | 1.274 | -4.758 | 38.858 | 1.00 | 23.84 | BLGL |
| ATOM | 778 | CD1 | TYR | 111 | 1.551 | -4.593 | 37.501 | 1.00 | 22.76 | BLGL |
| ATOM | 779 | CE1 | TYR | 111 | 0.878 | -3.641 | 36.742 | 1.00 | 23.56 | BLGL |
| ATOM | 780 | CD2 | TYR | 111 | 0.297 | -3.945 | 39.437 | 1.00 | 24.23 | BLGL |
| ATOM | 781 | CE2 | TYR | 111 | -0.378 | -2.991 | 38.688 | 1.00 | 23.70 | BLGL |
| ATOM | 782 | CZ | TYR | 111 | -0.082 | -2.844 | 37.344 | 1.00 | 23.27 | BLGL |
| ATOM | 783 | OH | TYR | 111 | -0.738 | -1.887 | 36.609 | 1.00 | 24.35 | BLGL |
| ATOM | 784 | C | TYR | 111 | 3.439 | -6.137 | 41.754 | 1.00 | 22.90 | BLGL |
| ATOM | 785 | O | TYR | 111 | 3.094 | -7.317 | 41.718 | 1.00 | 22.52 | BLGL |
| ATOM | 786 | N | SER | 112 | 4.372 | -5.668 | 42.574 | 1.00 | 22.56 | BLGL |
| ATOM | 787 | CA | SER | 112 | 5.071 | -6.493 | 43.544 | 1.00 | 22.63 | BLGL |
| ATOM | 788 | CB | SER | 112 | 6.249 | -7.201 | 42.892 | 1.00 | 22.37 | BLGL |
| ATOM | 789 | OG | SER | 112 | 7.002 | -7.894 | 43.866 | 1.00 | 23.73 | BLGL |
| ATOM | 790 | C | SER | 112 | 5.585 | -5.542 | 44.601 | 1.00 | 23.27 | BLGL |
| ATOM | 791 | O | SER | 112 | 5.631 | -4.333 | 44.368 | 1.00 | 24.65 | BLGL |

# Fig. 4 cont.

| ATOM | 792 | N   | ASP | 113 | 5.968  | -6.069  | 45.760 | 1.00 | 22.31 | BLGL |
|------|-----|-----|-----|-----|--------|---------|--------|------|-------|------|
| ATOM | 793 | CA  | ASP | 113 | 6.486  | -5.208  | 46.815 | 1.00 | 22.28 | BLGL |
| ATOM | 794 | CB  | ASP | 113 | 6.202  | -5.795  | 48.199 | 1.00 | 22.82 | BLGL |
| ATOM | 795 | CG  | ASP | 113 | 4.732  | -5.719  | 48.577 | 1.00 | 25.54 | BLGL |
| ATOM | 796 | OD1 | ASP | 113 | 4.032  | -4.825  | 48.056 | 1.00 | 23.47 | BLGL |
| ATOM | 797 | OD2 | ASP | 113 | 4.281  | -6.544  | 49.406 | 1.00 | 24.91 | BLGL |
| ATOM | 798 | C   | ASP | 113 | 7.982  | -4.969  | 46.651 | 1.00 | 21.86 | BLGL |
| ATOM | 799 | O   | ASP | 113 | 8.548  | -4.101  | 47.309 | 1.00 | 21.62 | BLGL |
| ATOM | 800 | N   | PHE | 114 | 8.622  | -5.738  | 45.775 | 1.00 | 20.23 | BLGL |
| ATOM | 801 | CA  | PHE | 114 | 10.046 | -5.563  | 45.547 | 1.00 | 20.78 | BLGL |
| ATOM | 802 | CB  | PHE | 114 | 10.853 | -6.387  | 46.549 | 1.00 | 21.28 | BLGL |
| ATOM | 803 | CG  | PHE | 114 | 12.221 | -5.822  | 46.838 | 1.00 | 24.03 | BLGL |
| ATOM | 804 | CD1 | PHE | 114 | 12.420 | -4.441  | 46.919 | 1.00 | 24.35 | BLGL |
| ATOM | 805 | CD2 | PHE | 114 | 13.308 | -6.666  | 47.064 | 1.00 | 24.49 | BLGL |
| ATOM | 806 | CE1 | PHE | 114 | 13.684 | -3.909  | 47.224 | 1.00 | 22.80 | BLGL |
| ATOM | 807 | CE2 | PHE | 114 | 14.575 | -6.144  | 47.372 | 1.00 | 20.26 | BLGL |
| ATOM | 808 | CZ  | PHE | 114 | 14.761 | -4.767  | 47.451 | 1.00 | 20.45 | BLGL |
| ATOM | 809 | C   | PHE | 114 | 10.392 | -5.952  | 44.122 | 1.00 | 21.41 | BLGL |
| ATOM | 810 | O   | PHE | 114 | 9.507  | -6.328  | 43.361 | 1.00 | 21.59 | BLGL |
| ATOM | 811 | N   | TRP | 115 | 11.675 | -5.856  | 43.768 | 1.00 | 20.29 | BLGL |
| ATOM | 812 | CA  | TRP | 115 | 12.152 | -6.160  | 42.418 | 1.00 | 19.28 | BLGL |
| ATOM | 813 | CB  | TRP | 115 | 13.634 | -6.577  | 42.445 | 1.00 | 20.57 | BLGL |
| ATOM | 814 | CG  | TRP | 115 | 14.575 | -5.534  | 42.963 | 1.00 | 21.03 | BLGL |
| ATOM | 815 | CD2 | TRP | 115 | 14.942 | -4.315  | 42.311 | 1.00 | 20.71 | BLGL |
| ATOM | 816 | CE2 | TRP | 115 | 15.786 | -3.607  | 43.198 | 1.00 | 21.97 | BLGL |
| ATOM | 817 | CE3 | TRP | 115 | 14.637 | -3.747  | 41.066 | 1.00 | 20.82 | BLGL |
| ATOM | 818 | CD1 | TRP | 115 | 15.202 | -5.523  | 44.177 | 1.00 | 19.55 | BLGL |
| ATOM | 819 | NE1 | TRP | 115 | 15.929 | -4.371  | 44.328 | 1.00 | 18.99 | BLGL |
| ATOM | 820 | CZ2 | TRP | 115 | 16.329 | -2.350  | 42.878 | 1.00 | 22.16 | BLGL |
| ATOM | 821 | CZ3 | TRP | 115 | 15.177 | -2.499  | 40.746 | 1.00 | 21.59 | BLGL |
| ATOM | 822 | CH2 | TRP | 115 | 16.013 | -1.815  | 41.653 | 1.00 | 22.47 | BLGL |
| ATOM | 823 | C   | TRP | 115 | 11.361 | -7.231  | 41.665 | 1.00 | 18.82 | BLGL |
| ATOM | 824 | O   | TRP | 115 | 11.090 | -8.308  | 42.193 | 1.00 | 17.18 | BLGL |
| ATOM | 825 | N   | ALA | 116 | 10.995 | -6.925  | 40.426 | 1.00 | 17.42 | BLGL |
| ATOM | 826 | CA  | ALA | 116 | 10.277 | -7.874  | 39.589 | 1.00 | 19.55 | BLGL |
| ATOM | 827 | CB  | ALA | 116 | 8.914  | -7.326  | 39.223 | 1.00 | 18.74 | BLGL |
| ATOM | 828 | C   | ALA | 116 | 11.110 | -8.105  | 38.331 | 1.00 | 22.25 | BLGL |
| ATOM | 829 | O   | ALA | 116 | 11.457 | -7.157  | 37.631 | 1.00 | 25.39 | BLGL |
| ATOM | 830 | N   | ASP | 117 | 11.450 | -9.358  | 38.051 | 1.00 | 21.71 | BLGL |
| ATOM | 831 | CA  | ASP | 117 | 12.243 | -9.672  | 36.872 | 1.00 | 22.29 | BLGL |
| ATOM | 832 | CB  | ASP | 117 | 13.736 | -9.620  | 37.209 | 1.00 | 22.60 | BLGL |
| ATOM | 833 | CG  | ASP | 117 | 14.124 | -10.578 | 38.309 | 1.00 | 26.69 | BLGL |
| ATOM | 834 | OD1 | ASP | 117 | 13.662 | -11.738 | 38.294 | 1.00 | 29.56 | BLGL |
| ATOM | 835 | OD2 | ASP | 117 | 14.907 | -10.171 | 39.190 | 1.00 | 30.52 | BLGL |
| ATOM | 836 | C   | ASP | 117 | 11.843 | -11.045 | 36.346 | 1.00 | 22.91 | BLGL |
| ATOM | 837 | O   | ASP | 117 | 10.840 | -11.601 | 36.784 | 1.00 | 24.06 | BLGL |
| ATOM | 838 | N   | PRO | 118 | 12.617 | -11.619 | 35.409 | 1.00 | 22.06 | BLGL |
| ATOM | 839 | CD  | PRO | 118 | 13.734 | -11.056 | 34.639 | 1.00 | 20.93 | BLGL |
| ATOM | 840 | CA  | PRO | 118 | 12.252 | -12.935 | 34.880 | 1.00 | 24.27 | BLGL |
| ATOM | 841 | CB  | PRO | 118 | 13.301 | -13.176 | 33.802 | 1.00 | 22.87 | BLGL |
| ATOM | 842 | CG  | PRO | 118 | 13.629 | -11.821 | 33.353 | 1.00 | 24.48 | BLGL |
| ATOM | 843 | C   | PRO | 118 | 12.202 | -14.077 | 35.884 | 1.00 | 26.00 | BLGL |
| ATOM | 844 | O   | PRO | 118 | 11.667 | -15.140 | 35.580 | 1.00 | 29.05 | BLGL |
| ATOM | 845 | N   | ALA | 119 | 12.755 | -13.868 | 37.071 | 1.00 | 28.00 | BLGL |
| ATOM | 846 | CA  | ALA | 119 | 12.762 | -14.917 | 38.086 | 1.00 | 28.48 | BLGL |
| ATOM | 847 | CB  | ALA | 119 | 14.186 | -15.188 | 38.543 | 1.00 | 27.97 | BLGL |
| ATOM | 848 | C   | ALA | 119 | 11.899 | -14.568 | 39.283 | 1.00 | 28.36 | BLGL |
| ATOM | 849 | O   | ALA | 119 | 11.407 | -15.447 | 39.981 | 1.00 | 30.80 | BLGL |
| ATOM | 850 | N   | LYS | 120 | 11.719 | -13.279 | 39.524 | 1.00 | 29.14 | BLGL |
| ATOM | 851 | CA  | LYS | 120 | 10.920 | -12.842 | 40.654 | 1.00 | 29.76 | BLGL |
| ATOM | 852 | CB  | LYS | 120 | 11.793 | -12.032 | 41.617 | 1.00 | 31.32 | BLGL |
| ATOM | 853 | CG  | LYS | 120 | 12.940 | -12.838 | 42.213 | 1.00 | 38.25 | BLGL |
| ATOM | 854 | CD  | LYS | 120 | 13.897 | -12.000 | 43.074 | 1.00 | 40.66 | BLGL |
| ATOM | 855 | CE  | LYS | 120 | 14.801 | -11.115 | 42.222 | 1.00 | 44.93 | BLGL |
| ATOM | 856 | NZ  | LYS | 120 | 15.827 | -10.373 | 43.027 | 1.00 | 46.70 | BLGL |
| ATOM | 857 | C   | LYS | 120 | 9.708  | -12.020 | 40.224 | 1.00 | 28.61 | BLGL |

# Fig. 4 cont.

| ATOM | 858 | O | LYS | 120 | 9.841 | -10.912 | 39.702 | 1.00 | 28.45 | BLGL |
|------|-----|-----|-----|-----|-------|---------|--------|------|-------|------|
| ATOM | 859 | N | GLN | 121 | 8.525 | -12.589 | 40.425 | 1.00 | 26.27 | BLGL |
| ATOM | 860 | CA | GLN | 121 | 7.273 | -11.913 | 40.108 | 1.00 | 25.49 | BLGL |
| ATOM | 861 | CB | GLN | 121 | 6.673 | -12.457 | 38.805 | 1.00 | 24.33 | BLGL |
| ATOM | 862 | CG | GLN | 121 | 7.392 | -12.034 | 37.525 | 1.00 | 20.53 | BLGL |
| ATOM | 863 | CD | GLN | 121 | 7.376 | -10.528 | 37.291 | 1.00 | 18.36 | BLGL |
| ATOM | 864 | OE1 | GLN | 121 | 6.425 | -9.838 | 37.659 | 1.00 | 15.80 | BLGL |
| ATOM | 865 | NE2 | GLN | 121 | 8.424 | -10.017 | 36.655 | 1.00 | 17.37 | BLGL |
| ATOM | 866 | C | GLN | 121 | 6.328 | -12.176 | 41.281 | 1.00 | 25.36 | BLGL |
| ATOM | 867 | O | GLN | 121 | 5.176 | -12.571 | 41.099 | 1.00 | 26.22 | BLGL |
| ATOM | 868 | N | LYS | 122 | 6.843 | -11.970 | 42.489 | 1.00 | 25.47 | BLGL |
| ATOM | 869 | CA | LYS | 122 | 6.091 | -12.188 | 43.716 | 1.00 | 25.96 | BLGL |
| ATOM | 870 | CB | LYS | 122 | 7.031 | -12.079 | 44.924 | 1.00 | 27.22 | BLGL |
| ATOM | 871 | CG | LYS | 122 | 6.394 | -12.412 | 46.260 | 1.00 | 29.39 | BLGL |
| ATOM | 872 | CD | LYS | 122 | 6.870 | -13.759 | 46.785 | 1.00 | 32.32 | BLGL |
| ATOM | 873 | CE | LYS | 122 | 7.832 | -13.609 | 47.961 | 1.00 | 31.56 | BLGL |
| ATOM | 874 | NZ | LYS | 122 | 7.187 | -12.997 | 49.160 | 1.00 | 32.62 | BLGL |
| ATOM | 875 | C | LYS | 122 | 4.968 | -11.162 | 43.833 | 1.00 | 26.53 | BLGL |
| ATOM | 876 | O | LYS | 122 | 5.151 | -9.988 | 43.504 | 1.00 | 28.15 | BLGL |
| ATOM | 877 | N | ALA | 123 | 3.804 | -11.603 | 44.298 | 1.00 | 25.34 | BLGL |
| ATOM | 878 | CA | ALA | 123 | 2.669 | -10.700 | 44.449 | 1.00 | 24.78 | BLGL |
| ATOM | 879 | CB | ALA | 123 | 1.377 | -11.491 | 44.559 | 1.00 | 24.09 | BLGL |
| ATOM | 880 | C | ALA | 123 | 2.830 | -9.820 | 45.675 | 1.00 | 23.46 | BLGL |
| ATOM | 881 | O | ALA | 123 | 3.519 | -10.177 | 46.622 | 1.00 | 23.28 | BLGL |
| ATOM | 882 | N | PRO | 124 | 2.212 | -8.636 | 45.660 | 1.00 | 23.79 | BLGL |
| ATOM | 883 | CD | PRO | 124 | 1.484 | -7.998 | 44.548 | 1.00 | 21.21 | BLGL |
| ATOM | 884 | CA | PRO | 124 | 2.310 | -7.738 | 46.811 | 1.00 | 22.77 | BLGL |
| ATOM | 885 | CB | PRO | 124 | 1.392 | -6.588 | 46.419 | 1.00 | 21.28 | BLGL |
| ATOM | 886 | CG | PRO | 124 | 1.521 | -6.547 | 44.927 | 1.00 | 19.51 | BLGL |
| ATOM | 887 | C | PRO | 124 | 1.791 | -8.491 | 48.037 | 1.00 | 23.09 | BLGL |
| ATOM | 888 | O | PRO | 124 | 0.883 | -9.312 | 47.922 | 1.00 | 22.17 | BLGL |
| ATOM | 889 | N | LYS | 125 | 2.360 | -8.228 | 49.205 | 1.00 | 25.24 | BLGL |
| ATOM | 890 | CA | LYS | 125 | 1.910 | -8.916 | 50.411 | 1.00 | 25.84 | BLGL |
| ATOM | 891 | CB | LYS | 125 | 2.612 | -8.350 | 51.656 | 1.00 | 23.65 | BLGL |
| ATOM | 892 | CG | LYS | 125 | 4.109 | -8.642 | 51.733 | 1.00 | 21.46 | BLGL |
| ATOM | 893 | CD | LYS | 125 | 4.750 | -8.067 | 52.990 | 1.00 | 15.25 | BLGL |
| ATOM | 894 | CE | LYS | 125 | 4.683 | -6.554 | 53.029 | 1.00 | 20.47 | BLGL |
| ATOM | 895 | NZ | LYS | 125 | 5.440 | -5.911 | 51.912 | 1.00 | 22.44 | BLGL |
| ATOM | 896 | C | LYS | 125 | 0.391 | -8.807 | 50.570 | 1.00 | 27.21 | BLGL |
| ATOM | 897 | O | LYS | 125 | -0.264 | -9.763 | 50.976 | 1.00 | 27.46 | BLGL |
| ATOM | 898 | N | ALA | 126 | -0.170 | -7.651 | 50.232 | 1.00 | 27.45 | BLGL |
| ATOM | 899 | CA | ALA | 126 | -1.608 | -7.438 | 50.360 | 1.00 | 28.44 | BLGL |
| ATOM | 900 | CB | ALA | 126 | -1.942 | -5.996 | 50.042 | 1.00 | 27.50 | BLGL |
| ATOM | 901 | C | ALA | 126 | -2.445 | -8.367 | 49.487 | 1.00 | 30.46 | BLGL |
| ATOM | 902 | O | ALA | 126 | -3.578 | -8.700 | 49.835 | 1.00 | 32.72 | BLGL |
| ATOM | 903 | N | TRP | 127 | -1.893 | -8.780 | 48.352 | 1.00 | 31.67 | BLGL |
| ATOM | 904 | CA | TRP | 127 | -2.608 | -9.663 | 47.436 | 1.00 | 32.34 | BLGL |
| ATOM | 905 | CB | TRP | 127 | -2.274 | -9.301 | 45.983 | 1.00 | 29.98 | BLGL |
| ATOM | 906 | CG | TRP | 127 | -2.525 | -7.864 | 45.623 | 1.00 | 26.78 | BLGL |
| ATOM | 907 | CD2 | TRP | 127 | -2.176 | -7.215 | 44.392 | 1.00 | 25.87 | BLGL |
| ATOM | 908 | CE2 | TRP | 127 | -2.582 | -5.869 | 44.499 | 1.00 | 24.64 | BLGL |
| ATOM | 909 | CE3 | TRP | 127 | -1.558 | -7.643 | 43.207 | 1.00 | 25.70 | BLGL |
| ATOM | 910 | CD1 | TRP | 127 | -3.116 | -6.913 | 46.400 | 1.00 | 25.22 | BLGL |
| ATOM | 911 | NE1 | TRP | 127 | -3.153 | -5.712 | 45.735 | 1.00 | 25.00 | BLGL |
| ATOM | 912 | CZ2 | TRP | 127 | -2.390 | -4.942 | 43.469 | 1.00 | 23.42 | BLGL |
| ATOM | 913 | CZ3 | TRP | 127 | -1.367 | -6.723 | 42.183 | 1.00 | 24.22 | BLGL |
| ATOM | 914 | CH2 | TRP | 127 | -1.781 | -5.387 | 42.323 | 1.00 | 24.78 | BLGL |
| ATOM | 915 | C | TRP | 127 | -2.220 | -11.113 | 47.694 | 1.00 | 34.48 | BLGL |
| ATOM | 916 | O | TRP | 127 | -2.786 | -12.039 | 47.101 | 1.00 | 34.45 | BLGL |
| ATOM | 917 | N | ALA | 128 | -1.244 | -11.284 | 48.585 | 1.00 | 37.15 | BLGL |
| ATOM | 918 | CA | ALA | 128 | -0.704 | -12.589 | 48.971 | 1.00 | 38.47 | BLGL |
| ATOM | 919 | CB | ALA | 128 | -0.198 | -12.528 | 50.396 | 1.00 | 40.00 | BLGL |
| ATOM | 920 | C | ALA | 128 | -1.663 | -13.759 | 48.817 | 1.00 | 39.10 | BLGL |
| ATOM | 921 | O | ALA | 128 | -1.406 | -14.671 | 48.032 | 1.00 | 38.72 | BLGL |
| ATOM | 922 | N | ASN | 129 | -2.754 | -13.751 | 49.574 | 1.00 | 40.50 | BLGL |
| ATOM | 923 | CA | ASN | 129 | -3.716 | -14.836 | 49.473 | 1.00 | 44.45 | BLGL |

## Fig. 4 cont.

| ATOM | 924 | CB | ASN | 129 | -3.794 | -15.632 | 50.788 | 1.00 | 47.42 | BLGL |
|------|-----|-----|-----|-----|--------|---------|--------|------|-------|------|
| ATOM | 925 | CG | ASN | 129 | -3.746 | -14.751 | 52.018 | 1.00 | 50.55 | BLGL |
| ATOM | 926 | OD1 | ASN | 129 | -3.975 | -13.545 | 51.941 | 1.00 | 54.24 | BLGL |
| ATOM | 927 | ND2 | ASN | 129 | -3.460 | -15.356 | 53.168 | 1.00 | 50.85 | BLGL |
| ATOM | 928 | C | ASN | 129 | -5.107 | -14.380 | 49.047 | 1.00 | 44.76 | BLGL |
| ATOM | 929 | O | ASN | 129 | -6.070 | -14.460 | 49.813 | 1.00 | 45.16 | BLGL |
| ATOM | 930 | N | LEU | 130 | -5.194 | -13.901 | 47.810 | 1.00 | 44.30 | BLGL |
| ATOM | 931 | CA | LEU | 130 | -6.452 | -13.456 | 47.230 | 1.00 | 43.76 | BLGL |
| ATOM | 932 | CB | LEU | 130 | -6.341 | -12.018 | 46.731 | 1.00 | 44.19 | BLGL |
| ATOM | 933 | CG | LEU | 130 | -6.396 | -10.901 | 47.767 | 1.00 | 44.74 | BLGL |
| ATOM | 934 | CD1 | LEU | 130 | -6.258 | -9.564 | 47.071 | 1.00 | 45.24 | BLGL |
| ATOM | 935 | CD2 | LEU | 130 | -7.712 | -10.970 | 48.515 | 1.00 | 45.37 | BLGL |
| ATOM | 936 | C | LEU | 130 | -6.727 | -14.363 | 46.049 | 1.00 | 43.61 | BLGL |
| ATOM | 937 | O | LEU | 130 | -5.801 | -14.769 | 45.351 | 1.00 | 43.36 | BLGL |
| ATOM | 938 | N | ASN | 131 | -7.991 | -14.695 | 45.823 | 1.00 | 44.12 | BLGL |
| ATOM | 939 | CA | ASN | 131 | -8.318 | -15.549 | 44.690 | 1.00 | 44.97 | BLGL |
| ATOM | 940 | CB | ASN | 131 | -9.757 | -16.078 | 44.801 | 1.00 | 47.76 | BLGL |
| ATOM | 941 | CG | ASN | 131 | -10.794 | -14.976 | 44.772 | 1.00 | 51.05 | BLGL |
| ATOM | 942 | OD1 | ASN | 131 | -10.669 | -13.968 | 45.465 | 1.00 | 55.52 | BLGL |
| ATOM | 943 | ND2 | ASN | 131 | -11.835 | -15.170 | 43.977 | 1.00 | 52.37 | BLGL |
| ATOM | 944 | C | ASN | 131 | -8.133 | -14.706 | 43.436 | 1.00 | 43.17 | BLGL |
| ATOM | 945 | O | ASN | 131 | -8.381 | -13.502 | 43.451 | 1.00 | 42.05 | BLGL |
| ATOM | 946 | N | PHE | 132 | -7.682 | -15.338 | 42.360 | 1.00 | 42.47 | BLGL |
| ATOM | 947 | CA | PHE | 132 | -7.440 | -14.638 | 41.107 | 1.00 | 42.04 | BLGL |
| ATOM | 948 | CB | PHE | 132 | -7.430 | -15.619 | 39.940 | 1.00 | 42.05 | BLGL |
| ATOM | 949 | CG | PHE | 132 | -7.126 | -14.971 | 38.633 | 1.00 | 42.75 | BLGL |
| ATOM | 950 | CD1 | PHE | 132 | -5.870 | -14.426 | 38.396 | 1.00 | 42.49 | BLGL |
| ATOM | 951 | CD2 | PHE | 132 | -8.103 | -14.855 | 37.656 | 1.00 | 43.76 | BLGL |
| ATOM | 952 | CE1 | PHE | 132 | -5.594 | -13.769 | 37.204 | 1.00 | 42.79 | BLGL |
| ATOM | 953 | CE2 | PHE | 132 | -7.834 | -14.197 | 36.455 | 1.00 | 44.60 | BLGL |
| ATOM | 954 | CZ | PHE | 132 | -6.579 | -13.655 | 36.232 | 1.00 | 43.31 | BLGL |
| ATOM | 955 | C | PHE | 132 | -8.439 | -13.523 | 40.808 | 1.00 | 41.68 | BLGL |
| ATOM | 956 | O | PHE | 132 | -8.050 | -12.415 | 40.445 | 1.00 | 41.50 | BLGL |
| ATOM | 957 | N | GLU | 133 | -9.725 | -13.815 | 40.951 | 1.00 | 42.52 | BLGL |
| ATOM | 958 | CA | GLU | 133 | -10.759 | -12.821 | 40.691 | 1.00 | 42.35 | BLGL |
| ATOM | 959 | CB | GLU | 133 | -12.138 | -13.409 | 40.985 | 1.00 | 46.23 | BLGL |
| ATOM | 960 | CG | GLU | 133 | -12.591 | -14.433 | 39.967 | 1.00 | 53.21 | BLGL |
| ATOM | 961 | CD | GLU | 133 | -12.550 | -13.879 | 38.553 | 1.00 | 57.33 | BLGL |
| ATOM | 962 | OE1 | GLU | 133 | -13.059 | -12.757 | 38.347 | 1.00 | 58.31 | BLGL |
| ATOM | 963 | OE2 | GLU | 133 | -12.015 | -14.564 | 37.652 | 1.00 | 61.34 | BLGL |
| ATOM | 964 | C | GLU | 133 | -10.573 | -11.542 | 41.500 | 1.00 | 40.12 | BLGL |
| ATOM | 965 | O | GLU | 133 | -10.654 | -10.443 | 40.951 | 1.00 | 38.25 | BLGL |
| ATOM | 966 | N | ASP | 134 | -10.326 | -11.691 | 42.800 | 1.00 | 38.18 | BLGL |
| ATOM | 967 | CA | ASP | 134 | -10.133 | -10.547 | 43.684 | 1.00 | 37.03 | BLGL |
| ATOM | 968 | CB | ASP | 134 | -10.203 | -10.994 | 45.142 | 1.00 | 39.68 | BLGL |
| ATOM | 969 | CG | ASP | 134 | -11.625 | -11.128 | 45.640 | 1.00 | 40.58 | BLGL |
| ATOM | 970 | OD1 | ASP | 134 | -11.816 | -11.683 | 46.744 | 1.00 | 40.76 | BLGL |
| ATOM | 971 | OD2 | ASP | 134 | -12.546 | -10.666 | 44.930 | 1.00 | 42.41 | BLGL |
| ATOM | 972 | C | ASP | 134 | -8.816 | -9.822 | 43.434 | 1.00 | 34.44 | BLGL |
| ATOM | 973 | O | ASP | 134 | -8.710 | -8.611 | 43.633 | 1.00 | 33.65 | BLGL |
| ATOM | 974 | N | LYS | 135 | -7.810 | -10.570 | 43.003 | 1.00 | 32.43 | BLGL |
| ATOM | 975 | CA | LYS | 135 | -6.510 | -9.989 | 42.717 | 1.00 | 30.17 | BLGL |
| ATOM | 976 | CB | LYS | 135 | -5.468 | -11.092 | 42.537 | 1.00 | 28.01 | BLGL |
| ATOM | 977 | CG | LYS | 135 | -4.058 | -10.568 | 42.377 | 1.00 | 25.79 | BLGL |
| ATOM | 978 | CD | LYS | 135 | -3.090 | -11.647 | 41.928 | 1.00 | 24.80 | BLGL |
| ATOM | 979 | CE | LYS | 135 | -2.994 | -12.773 | 42.922 | 1.00 | 24.10 | BLGL |
| ATOM | 980 | NZ | LYS | 135 | -1.961 | -13.742 | 42.491 | 1.00 | 24.21 | BLGL |
| ATOM | 981 | C | LYS | 135 | -6.615 | -9.147 | 41.443 | 1.00 | 29.06 | BLGL |
| ATOM | 982 | O | LYS | 135 | -6.092 | -8.032 | 41.384 | 1.00 | 29.12 | BLGL |
| ATOM | 983 | N | LYS | 136 | -7.303 | -9.682 | 40.436 | 1.00 | 28.19 | BLGL |
| ATOM | 984 | CA | LYS | 136 | -7.492 | -8.986 | 39.166 | 1.00 | 26.63 | BLGL |
| ATOM | 985 | CB | LYS | 136 | -8.364 | -9.819 | 38.220 | 1.00 | 28.55 | BLGL |
| ATOM | 986 | CG | LYS | 136 | -8.455 | -9.248 | 36.811 | 1.00 | 33.70 | BLGL |
| ATOM | 987 | CD | LYS | 136 | -9.739 | -9.661 | 36.093 | 1.00 | 40.26 | BLGL |
| ATOM | 988 | CE | LYS | 136 | -9.825 | -11.171 | 35.873 | 1.00 | 44.05 | BLGL |
| ATOM | 989 | NZ | LYS | 136 | -11.113 | -11.590 | 35.228 | 1.00 | 44.46 | BLGL |

# Fig. 4 cont.

| ATOM | 990 | C | LYS | 136 | -8.149 | -7.627 | 39.408 | 1.00 | 24.62 | BLGL |
|------|------|------|------|------|--------|--------|--------|------|-------|------|
| ATOM | 991 | O | LYS | 136 | -7.714 | -6.611 | 38.868 | 1.00 | 24.91 | BLGL |
| ATOM | 992 | N | THR | 137 | -9.197 | -7.607 | 40.221 | 1.00 | 23.73 | BLGL |
| ATOM | 993 | CA | THR | 137 | -9.874 | -6.356 | 40.519 | 1.00 | 24.53 | BLGL |
| ATOM | 994 | CB | THR | 137 | -11.262 | -6.603 | 41.168 | 1.00 | 26.21 | BLGL |
| ATOM | 995 | OG1 | THR | 137 | -11.679 | -5.422 | 41.855 | 1.00 | 28.27 | BLGL |
| ATOM | 996 | CG2 | THR | 137 | -11.220 | -7.759 | 42.134 | 1.00 | 27.71 | BLGL |
| ATOM | 997 | C | THR | 137 | -9.017 | -5.451 | 41.412 | 1.00 | 24.00 | BLGL |
| ATOM | 998 | O | THR | 137 | -9.108 | -4.221 | 41.334 | 1.00 | 23.13 | BLGL |
| ATOM | 999 | N | ALA | 138 | -8.174 | -6.054 | 42.248 | 1.00 | 22.08 | BLGL |
| ATOM | 1000 | CA | ALA | 138 | -7.289 | -5.277 | 43.115 | 1.00 | 23.30 | BLGL |
| ATOM | 1001 | CB | ALA | 138 | -6.612 | -6.182 | 44.128 | 1.00 | 19.73 | BLGL |
| ATOM | 1002 | C | ALA | 138 | -6.228 | -4.570 | 42.265 | 1.00 | 23.73 | BLGL |
| ATOM | 1003 | O | ALA | 138 | -5.896 | -3.401 | 42.497 | 1.00 | 23.84 | BLGL |
| ATOM | 1004 | N | LEU | 139 | -5.700 | -5.288 | 41.280 | 1.00 | 21.33 | BLGL |
| ATOM | 1005 | CA | LEU | 139 | -4.690 | -4.729 | 40.402 | 1.00 | 22.61 | BLGL |
| ATOM | 1006 | CB | LEU | 139 | -4.144 | -5.806 | 39.460 | 1.00 | 21.44 | BLGL |
| ATOM | 1007 | CG | LEU | 139 | -2.895 | -5.411 | 38.656 | 1.00 | 21.68 | BLGL |
| ATOM | 1008 | CD1 | LEU | 139 | -2.111 | -6.664 | 38.340 | 1.00 | 22.58 | BLGL |
| ATOM | 1009 | CD2 | LEU | 139 | -3.265 | -4.658 | 37.383 | 1.00 | 17.55 | BLGL |
| ATOM | 1010 | C | LEU | 139 | -5.280 | -3.576 | 39.603 | 1.00 | 23.36 | BLGL |
| ATOM | 1011 | O | LEU | 139 | -4.629 | -2.550 | 39.401 | 1.00 | 23.02 | BLGL |
| ATOM | 1012 | N | TYR | 140 | -6.513 | -3.747 | 39.141 | 1.00 | 24.62 | BLGL |
| ATOM | 1013 | CA | TYR | 140 | -7.176 | -2.697 | 38.381 | 1.00 | 25.60 | BLGL |
| ATOM | 1014 | CB | TYR | 140 | -8.514 | -3.206 | 37.833 | 1.00 | 23.98 | BLGL |
| ATOM | 1015 | CG | TYR | 140 | -9.494 | -2.109 | 37.498 | 1.00 | 22.17 | BLGL |
| ATOM | 1016 | CD1 | TYR | 140 | -10.389 | -1.634 | 38.452 | 1.00 | 25.15 | BLGL |
| ATOM | 1017 | CE1 | TYR | 140 | -11.259 | -0.580 | 38.167 | 1.00 | 25.77 | BLGL |
| ATOM | 1018 | CD2 | TYR | 140 | -9.492 | -1.508 | 36.247 | 1.00 | 22.26 | BLGL |
| ATOM | 1019 | CE2 | TYR | 140 | -10.353 | -0.457 | 35.950 | 1.00 | 24.44 | BLGL |
| ATOM | 1020 | CZ | TYR | 140 | -11.235 | 0.003 | 36.911 | 1.00 | 25.75 | BLGL |
| ATOM | 1021 | OH | TYR | 140 | -12.096 | 1.036 | 36.615 | 1.00 | 25.22 | BLGL |
| ATOM | 1022 | C | TYR | 140 | -7.393 | -1.468 | 39.272 | 1.00 | 27.76 | BLGL |
| ATOM | 1023 | O | TYR | 140 | -7.167 | -0.335 | 38.845 | 1.00 | 26.59 | BLGL |
| ATOM | 1024 | N | GLN | 141 | -7.828 | -1.698 | 40.508 | 1.00 | 29.36 | BLGL |
| ATOM | 1025 | CA | GLN | 141 | -8.061 | -0.605 | 41.446 | 1.00 | 31.47 | BLGL |
| ATOM | 1026 | CB | GLN | 141 | -8.645 | -1.134 | 42.758 | 1.00 | 34.45 | BLGL |
| ATOM | 1027 | CG | GLN | 141 | -10.105 | -1.525 | 42.664 | 1.00 | 44.36 | BLGL |
| ATOM | 1028 | CD | GLN | 141 | -11.015 | -0.331 | 42.408 | 1.00 | 49.85 | BLGL |
| ATOM | 1029 | OE1 | GLN | 141 | -12.161 | -0.487 | 41.957 | 1.00 | 52.06 | BLGL |
| ATOM | 1030 | NE2 | GLN | 141 | -10.515 | 0.870 | 42.707 | 1.00 | 49.83 | BLGL |
| ATOM | 1031 | C | GLN | 141 | -6.782 | 0.154 | 41.751 | 1.00 | 29.93 | BLGL |
| ATOM | 1032 | O | GLN | 141 | -6.751 | 1.387 | 41.698 | 1.00 | 28.20 | BLGL |
| ATOM | 1033 | N | TYR | 142 | -5.730 | -0.593 | 42.079 | 1.00 | 27.46 | BLGL |
| ATOM | 1034 | CA | TYR | 142 | -4.445 | -0.002 | 42.413 | 1.00 | 25.44 | BLGL |
| ATOM | 1035 | CB | TYR | 142 | -3.426 | -1.105 | 42.694 | 1.00 | 26.98 | BLGL |
| ATOM | 1036 | CG | TYR | 142 | -2.025 | -0.585 | 42.928 | 1.00 | 26.89 | BLGL |
| ATOM | 1037 | CD1 | TYR | 142 | -1.752 | 0.281 | 43.979 | 1.00 | 25.19 | BLGL |
| ATOM | 1038 | CE1 | TYR | 142 | -0.473 | 0.768 | 44.189 | 1.00 | 28.95 | BLGL |
| ATOM | 1039 | CD2 | TYR | 142 | -0.979 | -0.950 | 42.088 | 1.00 | 27.59 | BLGL |
| ATOM | 1040 | CE2 | TYR | 142 | 0.305 | -0.468 | 42.287 | 1.00 | 29.43 | BLGL |
| ATOM | 1041 | CZ | TYR | 142 | 0.553 | 0.390 | 43.341 | 1.00 | 30.68 | BLGL |
| ATOM | 1042 | OH | TYR | 142 | 1.829 | 0.862 | 43.554 | 1.00 | 32.86 | BLGL |
| ATOM | 1043 | C | TYR | 142 | -3.922 | 0.912 | 41.311 | 1.00 | 24.17 | BLGL |
| ATOM | 1044 | O | TYR | 142 | -3.466 | 2.026 | 41.572 | 1.00 | 22.37 | BLGL |
| ATOM | 1045 | N | THR | 143 | -3.988 | 0.432 | 40.076 | 1.00 | 23.95 | BLGL |
| ATOM | 1046 | CA | THR | 143 | -3.518 | 1.205 | 38.941 | 1.00 | 24.20 | BLGL |
| ATOM | 1047 | CB | THR | 143 | -3.626 | 0.397 | 37.649 | 1.00 | 22.46 | BLGL |
| ATOM | 1048 | OG1 | THR | 143 | -3.000 | -0.875 | 37.838 | 1.00 | 19.33 | BLGL |
| ATOM | 1049 | CG2 | THR | 143 | -2.948 | 1.129 | 36.508 | 1.00 | 20.23 | BLGL |
| ATOM | 1050 | C | THR | 143 | -4.361 | 2.459 | 38.803 | 1.00 | 25.95 | BLGL |
| ATOM | 1051 | O | THR | 143 | -3.836 | 3.568 | 38.689 | 1.00 | 27.54 | BLGL |
| ATOM | 1052 | N | LYS | 144 | -5.673 | 2.263 | 38.821 | 1.00 | 27.01 | BLGL |
| ATOM | 1053 | CA | LYS | 144 | -6.636 | 3.346 | 38.690 | 1.00 | 28.79 | BLGL |
| ATOM | 1054 | CB | LYS | 144 | -8.053 | 2.779 | 38.818 | 1.00 | 30.43 | BLGL |
| ATOM | 1055 | CG | LYS | 144 | -9.167 | 3.787 | 38.626 | 1.00 | 32.32 | BLGL |

# Fig. 4 cont.

| ATOM | 1056 | CD | LYS | 144 | -9.391 | 4.123 | 37.167 | 1.00 | 35.17 | BLGL |
|------|------|------|------|------|---------|--------|--------|------|-------|------|
| ATOM | 1057 | CE | LYS | 144 | -10.603 | 5.033 | 37.010 | 1.00 | 36.95 | BLGL |
| ATOM | 1058 | NZ | LYS | 144 | -11.835 | 4.435 | 37.605 | 1.00 | 37.88 | BLGL |
| ATOM | 1059 | C | LYS | 144 | -6.401 | 4.421 | 39.748 | 1.00 | 28.67 | BLGL |
| ATOM | 1060 | O | LYS | 144 | -6.322 | 5.606 | 39.433 | 1.00 | 29.09 | BLGL |
| ATOM | 1061 | N | GLN | 145 | -6.287 | 4.010 | 41.004 | 1.00 | 28.65 | BLGL |
| ATOM | 1062 | CA | GLN | 145 | -6.062 | 4.969 | 42.075 | 1.00 | 31.28 | BLGL |
| ATOM | 1063 | CB | GLN | 145 | -6.116 | 4.281 | 43.440 | 1.00 | 35.75 | BLGL |
| ATOM | 1064 | CG | GLN | 145 | -7.463 | 3.632 | 43.756 | 1.00 | 45.00 | BLGL |
| ATOM | 1065 | CD | GLN | 145 | -8.638 | 4.586 | 43.565 | 1.00 | 50.27 | BLGL |
| ATOM | 1066 | OE1 | GLN | 145 | -8.697 | 5.651 | 44.189 | 1.00 | 53.13 | BLGL |
| ATOM | 1067 | NE2 | GLN | 145 | -9.580 | 4.206 | 42.699 | 1.00 | 51.05 | BLGL |
| ATOM | 1068 | C | GLN | 145 | -4.720 | 5.666 | 41.905 | 1.00 | 30.73 | BLGL |
| ATOM | 1069 | O | GLN | 145 | -4.653 | 6.895 | 41.883 | 1.00 | 31.69 | BLGL |
| ATOM | 1070 | N | SER | 146 | -3.655 | 4.880 | 41.778 | 1.00 | 28.68 | BLGL |
| ATOM | 1071 | CA | SER | 146 | -2.315 | 5.429 | 41.614 | 1.00 | 27.00 | BLGL |
| ATOM | 1072 | CB | SER | 146 | -1.326 | 4.319 | 41.276 | 1.00 | 26.10 | BLGL |
| ATOM | 1073 | OG | SER | 146 | -1.175 | 3.432 | 42.363 | 1.00 | 25.05 | BLGL |
| ATOM | 1074 | C | SER | 146 | -2.258 | 6.485 | 40.529 | 1.00 | 26.20 | BLGL |
| ATOM | 1075 | O | SER | 146 | -1.733 | 7.576 | 40.739 | 1.00 | 24.18 | BLGL |
| ATOM | 1076 | N | LEU | 147 | -2.793 | 6.148 | 39.363 | 1.00 | 26.95 | BLGL |
| ATOM | 1077 | CA | LEU | 147 | -2.798 | 7.069 | 38.240 | 1.00 | 28.50 | BLGL |
| ATOM | 1078 | CB | LEU | 147 | -3.399 | 6.386 | 37.004 | 1.00 | 29.76 | BLGL |
| ATOM | 1079 | CG | LEU | 147 | -2.403 | 5.891 | 35.949 | 1.00 | 29.50 | BLGL |
| ATOM | 1080 | CD1 | LEU | 147 | -1.214 | 5.237 | 36.616 | 1.00 | 31.84 | BLGL |
| ATOM | 1081 | CD2 | LEU | 147 | -3.098 | 4.918 | 35.010 | 1.00 | 31.26 | BLGL |
| ATOM | 1082 | C | LEU | 147 | -3.554 | 8.352 | 38.563 | 1.00 | 28.49 | BLGL |
| ATOM | 1083 | O | LEU | 147 | -3.059 | 9.448 | 38.291 | 1.00 | 26.93 | BLGL |
| ATOM | 1084 | N | LYS | 148 | -4.740 | 8.227 | 39.156 | 1.00 | 29.43 | BLGL |
| ATOM | 1085 | CA | LYS | 148 | -5.520 | 9.412 | 39.485 | 1.00 | 32.08 | BLGL |
| ATOM | 1086 | CB | LYS | 148 | -6.897 | 9.041 | 40.039 | 1.00 | 35.85 | BLGL |
| ATOM | 1087 | CG | LYS | 148 | -7.879 | 10.208 | 39.955 | 1.00 | 44.89 | BLGL |
| ATOM | 1088 | CD | LYS | 148 | -9.276 | 9.854 | 40.430 | 1.00 | 48.80 | BLGL |
| ATOM | 1089 | CE | LYS | 148 | -9.319 | 9.641 | 41.939 | 1.00 | 53.72 | BLGL |
| ATOM | 1090 | NZ | LYS | 148 | -8.537 | 8.451 | 42.388 | 1.00 | 55.41 | BLGL |
| ATOM | 1091 | C | LYS | 148 | -4.772 | 10.277 | 40.488 | 1.00 | 30.09 | BLGL |
| ATOM | 1092 | O | LYS | 148 | -4.833 | 11.502 | 40.419 | 1.00 | 30.55 | BLGL |
| ATOM | 1093 | N | ALA | 149 | -4.063 | 9.636 | 41.412 | 1.00 | 27.72 | BLGL |
| ATOM | 1094 | CA | ALA | 149 | -3.279 | 10.352 | 42.411 | 1.00 | 27.90 | BLGL |
| ATOM | 1095 | CB | ALA | 149 | -2.623 | 9.367 | 43.368 | 1.00 | 26.54 | BLGL |
| ATOM | 1096 | C | ALA | 149 | -2.208 | 11.196 | 41.720 | 1.00 | 28.02 | BLGL |
| ATOM | 1097 | O | ALA | 149 | -1.981 | 12.357 | 42.075 | 1.00 | 27.39 | BLGL |
| ATOM | 1098 | N | MET | 150 | -1.547 | 10.607 | 40.729 | 1.00 | 27.66 | BLGL |
| ATOM | 1099 | CA | MET | 150 | -0.511 | 11.319 | 39.996 | 1.00 | 28.87 | BLGL |
| ATOM | 1100 | CB | MET | 150 | 0.228 | 10.357 | 39.063 | 1.00 | 28.84 | BLGL |
| ATOM | 1101 | CG | MET | 150 | 1.084 | 9.358 | 39.828 | 1.00 | 31.73 | BLGL |
| ATOM | 1102 | SD | MET | 150 | 2.122 | 8.307 | 38.803 | 1.00 | 34.53 | BLGL |
| ATOM | 1103 | CE | MET | 150 | 1.218 | 6.808 | 38.827 | 1.00 | 36.46 | BLGL |
| ATOM | 1104 | C | MET | 150 | -1.101 | 12.491 | 39.219 | 1.00 | 28.60 | BLGL |
| ATOM | 1105 | O | MET | 150 | -0.518 | 13.575 | 39.167 | 1.00 | 25.71 | BLGL |
| ATOM | 1106 | N | LYS | 151 | -2.269 | 12.274 | 38.626 | 1.00 | 30.33 | BLGL |
| ATOM | 1107 | CA | LYS | 151 | -2.939 | 13.327 | 37.871 | 1.00 | 31.72 | BLGL |
| ATOM | 1108 | CB | LYS | 151 | -4.229 | 12.793 | 37.254 | 1.00 | 32.47 | BLGL |
| ATOM | 1109 | CG | LYS | 151 | -4.036 | 12.005 | 35.980 | 1.00 | 35.00 | BLGL |
| ATOM | 1110 | CD | LYS | 151 | -3.833 | 12.927 | 34.789 | 1.00 | 38.64 | BLGL |
| ATOM | 1111 | CE | LYS | 151 | -3.939 | 12.159 | 33.477 | 1.00 | 40.97 | BLGL |
| ATOM | 1112 | NZ | LYS | 151 | -3.816 | 13.050 | 32.295 | 1.00 | 40.80 | BLGL |
| ATOM | 1113 | C | LYS | 151 | -3.261 | 14.501 | 38.787 | 1.00 | 31.68 | BLGL |
| ATOM | 1114 | O | LYS | 151 | -3.008 | 15.655 | 38.442 | 1.00 | 32.97 | BLGL |
| ATOM | 1115 | N | ALA | 152 | -3.823 | 14.199 | 39.953 | 1.00 | 31.23 | BLGL |
| ATOM | 1116 | CA | ALA | 152 | -4.176 | 15.228 | 40.921 | 1.00 | 30.30 | BLGL |
| ATOM | 1117 | CB | ALA | 152 | -4.759 | 14.590 | 42.185 | 1.00 | 29.61 | BLGL |
| ATOM | 1118 | C | ALA | 152 | -2.952 | 16.057 | 41.273 | 1.00 | 29.37 | BLGL |
| ATOM | 1119 | O | ALA | 152 | -3.066 | 17.247 | 41.544 | 1.00 | 30.53 | BLGL |
| ATOM | 1120 | N | ALA | 153 | -1.783 | 15.425 | 41.272 | 1.00 | 29.04 | BLGL |
| ATOM | 1121 | CA | ALA | 153 | -0.543 | 16.124 | 41.596 | 1.00 | 29.10 | BLGL |

# Fig. 4 cont.

| ATOM | 1122 | CB  | ALA | 153 | 0.517  | 15.134 | 42.032 | 1.00 | 30.13 | BLGL |
|------|------|-----|-----|-----|--------|--------|--------|------|-------|------|
| ATOM | 1123 | C   | ALA | 153 | -0.056 | 16.910 | 40.391 | 1.00 | 29.10 | BLGL |
| ATOM | 1124 | O   | ALA | 153 | 0.990  | 17.561 | 40.435 | 1.00 | 29.45 | BLGL |
| ATOM | 1125 | N   | GLY | 154 | -0.824 | 16.835 | 39.310 | 1.00 | 28.65 | BLGL |
| ATOM | 1126 | CA  | GLY | 154 | -0.482 | 17.557 | 38.101 | 1.00 | 26.76 | BLGL |
| ATOM | 1127 | C   | GLY | 154 | 0.711  | 17.017 | 37.340 | 1.00 | 26.93 | BLGL |
| ATOM | 1128 | O   | GLY | 154 | 1.406  | 17.770 | 36.661 | 1.00 | 25.28 | BLGL |
| ATOM | 1129 | N   | ILE | 155 | 0.948  | 15.713 | 37.444 | 1.00 | 27.10 | BLGL |
| ATOM | 1130 | CA  | ILE | 155 | 2.064  | 15.080 | 36.745 | 1.00 | 25.61 | BLGL |
| ATOM | 1131 | CB  | ILE | 155 | 2.532  | 13.809 | 37.496 | 1.00 | 24.73 | BLGL |
| ATOM | 1132 | CG2 | ILE | 155 | 3.661  | 13.118 | 36.724 | 1.00 | 23.73 | BLGL |
| ATOM | 1133 | CG1 | ILE | 155 | 2.985  | 14.196 | 38.907 | 1.00 | 22.31 | BLGL |
| ATOM | 1134 | CD1 | ILE | 155 | 3.188  | 13.018 | 39.842 | 1.00 | 21.74 | BLGL |
| ATOM | 1135 | C   | ILE | 155 | 1.672  | 14.723 | 35.306 | 1.00 | 24.09 | BLGL |
| ATOM | 1136 | O   | ILE | 155 | 0.568  | 14.240 | 35.056 | 1.00 | 25.01 | BLGL |
| ATOM | 1137 | N   | ASP | 156 | 2.581  | 14.975 | 34.369 | 1.00 | 21.70 | BLGL |
| ATOM | 1138 | CA  | ASP | 156 | 2.354  | 14.695 | 32.959 | 1.00 | 23.92 | BLGL |
| ATOM | 1139 | CB  | ASP | 156 | 3.172  | 15.657 | 32.089 | 1.00 | 26.46 | BLGL |
| ATOM | 1140 | CG  | ASP | 156 | 2.889  | 15.486 | 30.602 | 1.00 | 30.77 | BLGL |
| ATOM | 1141 | OD1 | ASP | 156 | 3.579  | 16.140 | 29.792 | 1.00 | 33.81 | BLGL |
| ATOM | 1142 | OD2 | ASP | 156 | 1.976  | 14.706 | 30.239 | 1.00 | 32.30 | BLGL |
| ATOM | 1143 | C   | ASP | 156 | 2.757  | 13.261 | 32.644 | 1.00 | 23.58 | BLGL |
| ATOM | 1144 | O   | ASP | 156 | 3.904  | 12.986 | 32.319 | 1.00 | 26.10 | BLGL |
| ATOM | 1145 | N   | ILE | 157 | 1.805  | 12.348 | 32.750 | 1.00 | 22.55 | BLGL |
| ATOM | 1146 | CA  | ILE | 157 | 2.062  | 10.945 | 32.484 | 1.00 | 21.98 | BLGL |
| ATOM | 1147 | CB  | ILE | 157 | 1.070  | 10.058 | 33.254 | 1.00 | 22.84 | BLGL |
| ATOM | 1148 | CG2 | ILE | 157 | 1.368  | 8.595  | 32.990 | 1.00 | 18.93 | BLGL |
| ATOM | 1149 | CG1 | ILE | 157 | 1.137  | 10.385 | 34.744 | 1.00 | 23.81 | BLGL |
| ATOM | 1150 | CD1 | ILE | 157 | -0.082 | 9.922  | 35.514 | 1.00 | 26.52 | BLGL |
| ATOM | 1151 | C   | ILE | 157 | 1.894  | 10.675 | 30.997 | 1.00 | 20.48 | BLGL |
| ATOM | 1152 | O   | ILE | 157 | 0.819  | 10.885 | 30.443 | 1.00 | 22.51 | BLGL |
| ATOM | 1153 | N   | GLY | 158 | 2.950  | 10.207 | 30.349 | 1.00 | 18.57 | BLGL |
| ATOM | 1154 | CA  | GLY | 158 | 2.847  | 9.927  | 28.935 | 1.00 | 16.55 | BLGL |
| ATOM | 1155 | C   | GLY | 158 | 2.758  | 8.445  | 28.632 | 1.00 | 17.26 | BLGL |
| ATOM | 1156 | O   | GLY | 158 | 2.227  | 8.042  | 27.599 | 1.00 | 17.93 | BLGL |
| ATOM | 1157 | N   | MET | 159 | 3.245  | 7.622  | 29.550 | 1.00 | 18.71 | BLGL |
| ATOM | 1158 | CA  | MET | 159 | 3.260  | 6.186  | 29.322 | 1.00 | 19.00 | BLGL |
| ATOM | 1159 | CB  | MET | 159 | 4.559  | 5.834  | 28.588 | 1.00 | 17.91 | BLGL |
| ATOM | 1160 | CG  | MET | 159 | 4.563  | 4.506  | 27.872 | 1.00 | 24.08 | BLGL |
| ATOM | 1161 | SD  | MET | 159 | 6.139  | 4.187  | 27.000 | 1.00 | 30.17 | BLGL |
| ATOM | 1162 | CE  | MET | 159 | 6.095  | 5.442  | 25.740 | 1.00 | 26.74 | BLGL |
| ATOM | 1163 | C   | MET | 159 | 3.156  | 5.395  | 30.630 | 1.00 | 19.17 | BLGL |
| ATOM | 1164 | O   | MET | 159 | 3.573  | 5.855  | 31.696 | 1.00 | 16.99 | BLGL |
| ATOM | 1165 | N   | VAL | 160 | 2.579  | 4.204  | 30.543 | 1.00 | 18.21 | BLGL |
| ATOM | 1166 | CA  | VAL | 160 | 2.450  | 3.345  | 31.707 | 1.00 | 17.42 | BLGL |
| ATOM | 1167 | CB  | VAL | 160 | 1.002  | 3.285  | 32.245 | 1.00 | 17.75 | BLGL |
| ATOM | 1168 | CG1 | VAL | 160 | 0.920  | 2.287  | 33.384 | 1.00 | 16.21 | BLGL |
| ATOM | 1169 | CG2 | VAL | 160 | 0.570  | 4.654  | 32.739 | 1.00 | 18.60 | BLGL |
| ATOM | 1170 | C   | VAL | 160 | 2.891  | 1.944  | 31.332 | 1.00 | 17.12 | BLGL |
| ATOM | 1171 | O   | VAL | 160 | 2.516  | 1.406  | 30.292 | 1.00 | 17.78 | BLGL |
| ATOM | 1172 | N   | GLN | 161 | 3.704  | 1.360  | 32.192 | 1.00 | 17.31 | BLGL |
| ATOM | 1173 | CA  | GLN | 161 | 4.211  | 0.028  | 31.963 | 1.00 | 17.58 | BLGL |
| ATOM | 1174 | CB  | GLN | 161 | 5.709  | 0.018  | 32.272 | 1.00 | 17.55 | BLGL |
| ATOM | 1175 | CG  | GLN | 161 | 6.446  | -1.213 | 31.826 | 1.00 | 16.31 | BLGL |
| ATOM | 1176 | CD  | GLN | 161 | 7.935  | -1.106 | 32.056 | 1.00 | 16.53 | BLGL |
| ATOM | 1177 | OE1 | GLN | 161 | 8.570  | -0.132 | 31.641 | 1.00 | 17.05 | BLGL |
| ATOM | 1178 | NE2 | GLN | 161 | 8.508  | -2.114 | 32.707 | 1.00 | 12.70 | BLGL |
| ATOM | 1179 | C   | GLN | 161 | 3.439  | -0.903 | 32.893 | 1.00 | 16.74 | BLGL |
| ATOM | 1180 | O   | GLN | 161 | 3.455  | -0.719 | 34.106 | 1.00 | 17.03 | BLGL |
| ATOM | 1181 | N   | VAL | 162 | 2.736  | -1.882 | 32.330 | 1.00 | 14.93 | BLGL |
| ATOM | 1182 | CA  | VAL | 162 | 1.975  | -2.818 | 33.153 | 1.00 | 14.33 | BLGL |
| ATOM | 1183 | CB  | VAL | 162 | 0.648  | -3.209 | 32.455 | 1.00 | 14.98 | BLGL |
| ATOM | 1184 | CG1 | VAL | 162 | -0.143 | -4.195 | 33.304 | 1.00 | 12.90 | BLGL |
| ATOM | 1185 | CG2 | VAL | 162 | -0.176 | -1.964 | 32.213 | 1.00 | 12.73 | BLGL |
| ATOM | 1186 | C   | VAL | 162 | 2.840  | -4.051 | 33.411 | 1.00 | 15.01 | BLGL |
| ATOM | 1187 | O   | VAL | 162 | 2.763  | -5.046 | 32.691 | 1.00 | 15.57 | BLGL |

# Fig. 4 cont.

| ATOM | 1188 | N | GLY | 163 | 3.674 | -3.965 | 34.444 | 1.00 | 13.93 | BLGL |
|------|------|------|-----|------|--------|---------|--------|------|-------|------|
| ATOM | 1189 | CA | GLY | 163 | 4.568 | -5.062 | 34.765 | 1.00 | 16.33 | BLGL |
| ATOM | 1190 | C | GLY | 163 | 6.001 | -4.755 | 34.350 | 1.00 | 17.03 | BLGL |
| ATOM | 1191 | O | GLY | 163 | 6.239 | -3.875 | 33.521 | 1.00 | 17.31 | BLGL |
| ATOM | 1192 | N | ASN | 164 | 6.958 | -5.485 | 34.917 | 1.00 | 17.42 | BLGL |
| ATOM | 1193 | CA | ASN | 164 | 8.374 | -5.274 | 34.628 | 1.00 | 16.23 | BLGL |
| ATOM | 1194 | CB | ASN | 164 | 9.035 | -4.629 | 35.845 | 1.00 | 13.47 | BLGL |
| ATOM | 1195 | CG | ASN | 164 | 10.413 | -4.117 | 35.556 | 1.00 | 11.45 | BLGL |
| ATOM | 1196 | OD1 | ASN | 164 | 10.581 | -3.019 | 35.026 | 1.00 | 13.59 | BLGL |
| ATOM | 1197 | ND2 | ASN | 164 | 11.416 | -4.912 | 35.889 | 1.00 | 11.01 | BLGL |
| ATOM | 1198 | C | ASN | 164 | 9.051 | -6.614 | 34.315 | 1.00 | 17.48 | BLGL |
| ATOM | 1199 | O | ASN | 164 | 9.131 | -7.490 | 35.175 | 1.00 | 19.59 | BLGL |
| ATOM | 1200 | N | GLU | 165 | 9.537 | -6.765 | 33.085 | 1.00 | 17.58 | BLGL |
| ATOM | 1201 | CA | GLU | 165 | 10.197 | -7.998 | 32.643 | 1.00 | 17.54 | BLGL |
| ATOM | 1202 | CB | GLU | 165 | 11.605 | -8.093 | 33.244 | 1.00 | 16.33 | BLGL |
| ATOM | 1203 | CG | GLU | 165 | 12.467 | -6.875 | 32.940 | 1.00 | 17.40 | BLGL |
| ATOM | 1204 | CD | GLU | 165 | 13.938 | -7.095 | 33.223 | 1.00 | 17.97 | BLGL |
| ATOM | 1205 | OE1 | GLU | 165 | 14.260 | -7.739 | 34.236 | 1.00 | 20.07 | BLGL |
| ATOM | 1206 | OE2 | GLU | 165 | 14.783 | -6.613 | 32.442 | 1.00 | 15.79 | BLGL |
| ATOM | 1207 | C | GLU | 165 | 9.372 | -9.248 | 32.982 | 1.00 | 16.57 | BLGL |
| ATOM | 1208 | O | GLU | 165 | 9.875 | -10.221 | 33.534 | 1.00 | 14.22 | BLGL |
| ATOM | 1209 | N | THR | 166 | 8.094 | -9.196 | 32.618 | 1.00 | 16.92 | BLGL |
| ATOM | 1210 | CA | THR | 166. | 7.146 | -10.267 | 32.860 | 1.00 | 15.12 | BLGL |
| ATOM | 1211 | CB | THR | 166 | 5.723 | -9.713 | 32.782 | 1.00 | 17.38 | BLGL |
| ATOM | 1212 | OG1 | THR | 166 | 5.514 | -9.130 | 31.490 | 1.00 | 16.95 | BLGL |
| ATOM | 1213 | CG2 | THR | 166 | 5.511 | -8.629 | 33.850 | 1.00 | 17.63 | BLGL |
| ATOM | 1214 | C | THR | 166 | 7.304 | -11.411 | 31.860 | 1.00 | 15.92 | BLGL |
| ATOM | 1215 | O | THR | 166 | 6.380 | -11.741 | 31.131 | 1.00 | 13.18 | BLGL |
| ATOM | 1216 | N | ASN | 167 | 8.488 | -12.013 | 31.835 | 1.00 | 18.90 | BLGL |
| ATOM | 1217 | CA | ASN | 167 | 8.775 | -13.122 | 30.933 | 1.00 | 19.84 | BLGL |
| ATOM | 1218 | CB | ASN | 167 | 10.277 | -13.399 | 30.885 | 1.00 | 19.56 | BLGL |
| ATOM | 1219 | CG | ASN | 167 | 11.014 | -12.455 | 29.974 | 1.00 | 19.68 | BLGL |
| ATOM | 1220 | OD1 | ASN | 167 | 10.597 | -11.320 | 29.774 | 1.00 | 21.70 | BLGL |
| ATOM | 1221 | ND2 | ASN | 167 | 12.132 | -12.912 | 29.429 | 1.00 | 19.90 | BLGL |
| ATOM | 1222 | C | ASN | 167 | 8.074 | -14.397 | 31.343 | 1.00 | 20.80 | BLGL |
| ATOM | 1223 | O | ASN | 167 | 7.670 | -15.175 | 30.489 | 1.00 | 22.87 | BLGL |
| ATOM | 1224 | N | GLY | 168 | 7.936 | -14.615 | 32.647 | 1.00 | 22.03 | BLGL |
| ATOM | 1225 | CA | GLY | 168 | 7.302 | -15.833 | 33.114 | 1.00 | 24.61 | BLGL |
| ATOM | 1226 | C | GLY | 168 | 6.216 | -15.699 | 34.164 | 1.00 | 26.99 | BLGL |
| ATOM | 1227 | O | GLY | 168 | 5.663 | -16.702 | 34.620 | 1.00 | 28.98 | BLGL |
| ATOM | 1228 | N | GLY | 169 | 5.898 | -14.478 | 34.562 | 1.00 | 26.63 | BLGL |
| ATOM | 1229 | CA | GLY | 169 | 4.865 | -14.319 | 35.558 | 1.00 | 25.86 | BLGL |
| ATOM | 1230 | C | GLY | 169 | 4.516 | -12.878 | 35.831 | 1.00 | 27.02 | BLGL |
| ATOM | 1231 | O | GLY | 169 | 5.166 | -11.959 | 35.334 | 1.00 | 28.44 | BLGL |
| ATOM | 1232 | N | LEU | 170 | 3.467 | -12.691 | 36.622 | 1.00 | 26.37 | BLGL |
| ATOM | 1233 | CA | LEU | 170 | 2.996 | -11.371 | 37.005 | 1.00 | 23.73 | BLGL |
| ATOM | 1234 | CB | LEU | 170 | 2.164 | -10.751 | 35.875 | 1.00 | 20.57 | BLGL |
| ATOM | 1235 | CG | LEU | 170 | 1.474 | -9.415 | 36.185 | 1.00 | 21.09 | BLGL |
| ATOM | 1236 | CD1 | LEU | 170 | 2.470 | -8.395 | 36.723 | 1.00 | 21.42 | BLGL |
| ATOM | 1237 | CD2 | LEU | 170 | 0.811 | -8.894 | 34.934 | 1.00 | 20.49 | BLGL |
| ATOM | 1238 | C | LEU | 170 | 2.158 | -11.504 | 38.272 | 1.00 | 23.90 | BLGL |
| ATOM | 1239 | O | LEU | 170 | 1.222 | -12.305 | 38.326 | 1.00 | 22.71 | BLGL |
| ATOM | 1240 | N | ALA | 171 | 2.522 | -10.731 | 39.292 | 1.00 | 23.01 | BLGL |
| ATOM | 1241 | CA | ALA | 171 | 1.816 | -10.724 | 40.567 | 1.00 | 22.14 | BLGL |
| ATOM | 1242 | CB | ALA | 171 | 0.544 | -9.911 | 40.433 | 1.00 | 22.04 | BLGL |
| ATOM | 1243 | C | ALA | 171 | 1.488 | -12.114 | 41.109 | 1.00 | 23.55 | BLGL |
| ATOM | 1244 | O | ALA | 171 | 0.354 | -12.382 | 41.512 | 1.00 | 23.66 | BLGL |
| ATOM | 1245 | N | GLY | 172 | 2.479 | -12.996 | 41.122 | 1.00 | 22.96 | BLGL |
| ATOM | 1246 | CA | GLY | 172 | 2.259 | -14.337 | 41.632 | 1.00 | 25.97 | BLGL |
| ATOM | 1247 | C | GLY | 172 | 1.592 | -15.299 | 40.666 | 1.00 | 27.36 | BLGL |
| ATOM | 1248 | O | GLY | 172 | 1.412 | -16.474 | 40.980 | 1.00 | 27.94 | BLGL |
| ATOM | 1249 | N | GLU | 173 | 1.225 | -14.808 | 39.490 | 1.00 | 28.30 | BLGL |
| ATOM | 1250 | CA | GLU | 173 | 0.584 | -15.643 | 38.487 | 1.00 | 29.90 | BLGL |
| ATOM | 1251 | CB | GLU | 173 | -0.540 | -14.858 | 37.815 | 1.00 | 30.87 | BLGL |
| ATOM | 1252 | CG | GLU | 173 | -1.888 | -15.557 | 37.824 | 1.00 | 33.63 | BLGL |
| ATOM | 1253 | CD | GLU | 173 | -2.308 | -16.014 | 39.208 | 1.00 | 34.41 | BLGL |

# Fig. 4 cont.

| | | | | | | | | | |
|------|------|-----|-----|-----|---------|---------|--------|------|-------|------|
| ATOM | 1254 | OE1 | GLU | 173 | -2.334 | -15.181 | 40.139 | 1.00 | 34.20 | BLGL |
| ATOM | 1255 | OE2 | GLU | 173 | -2.618 | -17.214 | 39.359 | 1.00 | 34.57 | BLGL |
| ATOM | 1256 | C   | GLU | 173 | 1.619  | -16.084 | 37.450 | 1.00 | 30.77 | BLGL |
| ATOM | 1257 | O   | GLU | 173 | 2.481  | -15.302 | 37.053 | 1.00 | 31.69 | BLGL |
| ATOM | 1258 | N   | THR | 174 | 1.539  | -17.338 | 37.017 | 1.00 | 30.71 | BLGL |
| ATOM | 1259 | CA  | THR | 174 | 2.484  | -17.864 | 36.038 | 1.00 | 30.81 | BLGL |
| ATOM | 1260 | CB  | THR | 174 | 3.366  | -18.975 | 36.661 | 1.00 | 30.70 | BLGL |
| ATOM | 1261 | OG1 | THR | 174 | 2.533  | -20.027 | 37.167 | 1.00 | 33.92 | BLGL |
| ATOM | 1262 | CG2 | THR | 174 | 4.201  | -18.416 | 37.792 | 1.00 | 29.44 | BLGL |
| ATOM | 1263 | C   | THR | 174 | 1.801  | -18.426 | 34.792 | 1.00 | 31.23 | BLGL |
| ATOM | 1264 | O   | THR | 174 | 2.470  | -18.868 | 33.857 | 1.00 | 31.14 | BLGL |
| ATOM | 1265 | N   | ASP | 175 | 0.473  | -18.409 | 34.779 | 1.00 | 31.31 | BLGL |
| ATOM | 1266 | CA  | ASP | 175 | -0.276 | -18.923 | 33.640 | 1.00 | 31.53 | BLGL |
| ATOM | 1267 | CB  | ASP | 175 | -1.565 | -19.589 | 34.120 | 1.00 | 35.17 | BLGL |
| ATOM | 1268 | CG  | ASP | 175 | -2.447 | -20.030 | 32.972 | 1.00 | 38.71 | BLGL |
| ATOM | 1269 | OD1 | ASP | 175 | -1.925 | -20.654 | 32.023 | 1.00 | 39.79 | BLGL |
| ATOM | 1270 | OD2 | ASP | 175 | -3.665 | -19.758 | 33.022 | 1.00 | 42.47 | BLGL |
| ATOM | 1271 | C   | ASP | 175 | -0.605 | -17.796 | 32.674 | 1.00 | 30.63 | BLGL |
| ATOM | 1272 | O   | ASP | 175 | -1.363 | -16.890 | 33.016 | 1.00 | 30.64 | BLGL |
| ATOM | 1273 | N   | TRP | 176 | -0.055 | -17.861 | 31.463 | 1.00 | 27.62 | BLGL |
| ATOM | 1274 | CA  | TRP | 176 | -0.281 | -16.806 | 30.480 | 1.00 | 27.93 | BLGL |
| ATOM | 1275 | CB  | TRP | 176 | 0.403  | -17.147 | 29.157 | 1.00 | 24.63 | BLGL |
| ATOM | 1276 | CG  | TRP | 176 | 1.882  | -16.910 | 29.193 | 1.00 | 26.55 | BLGL |
| ATOM | 1277 | CD2 | TRP | 176 | 2.557  | -15.666 | 28.966 | 1.00 | 27.36 | BLGL |
| ATOM | 1278 | CE2 | TRP | 176 | 3.940  | -15.900 | 29.148 | 1.00 | 27.27 | BLGL |
| ATOM | 1279 | CE3 | TRP | 176 | 2.128  | -14.375 | 28.625 | 1.00 | 27.01 | BLGL |
| ATOM | 1280 | CD1 | TRP | 176 | 2.855  | -17.820 | 29.498 | 1.00 | 26.56 | BLGL |
| ATOM | 1281 | NE1 | TRP | 176 | 4.094  | -17.222 | 29.473 | 1.00 | 26.37 | BLGL |
| ATOM | 1282 | CZ2 | TRP | 176 | 4.899  | -14.887 | 29.004 | 1.00 | 25.56 | BLGL |
| ATOM | 1283 | CZ3 | TRP | 176 | 3.085  | -13.365 | 28.482 | 1.00 | 25.94 | BLGL |
| ATOM | 1284 | CH2 | TRP | 176 | 4.453  | -13.631 | 28.671 | 1.00 | 25.57 | BLGL |
| ATOM | 1285 | C   | TRP | 176 | -1.739 | -16.427 | 30.234 | 1.00 | 29.80 | BLGL |
| ATOM | 1286 | O   | TRP | 176 | -2.033 | -15.289 | 29.857 | 1.00 | 30.42 | BLGL |
| ATOM | 1287 | N   | ALA | 177 | -2.656 | -17.368 | 30.441 | 1.00 | 31.37 | BLGL |
| ATOM | 1288 | CA  | ALA | 177 | -4.073 | -17.077 | 30.249 | 1.00 | 30.31 | BLGL |
| ATOM | 1289 | CB  | ALA | 177 | -4.889 | -18.354 | 30.339 | 1.00 | 30.40 | BLGL |
| ATOM | 1290 | C   | ALA | 177 | -4.500 | -16.104 | 31.342 | 1.00 | 31.32 | BLGL |
| ATOM | 1291 | O   | ALA | 177 | -5.199 | -15.124 | 31.085 | 1.00 | 31.10 | BLGL |
| ATOM | 1292 | N   | LYS | 178 | -4.070 | -16.379 | 32.569 | 1.00 | 30.35 | BLGL |
| ATOM | 1293 | CA  | LYS | 178 | -4.401 | -15.507 | 33.680 | 1.00 | 31.58 | BLGL |
| ATOM | 1294 | CB  | LYS | 178 | -4.181 | -16.235 | 35.008 | 1.00 | 33.69 | BLGL |
| ATOM | 1295 | CG  | LYS | 178 | -5.114 | -17.410 | 35.234 | 1.00 | 37.35 | BLGL |
| ATOM | 1296 | CD  | LYS | 178 | -4.994 | -17.911 | 36.664 | 1.00 | 43.39 | BLGL |
| ATOM | 1297 | CE  | LYS | 178 | -5.780 | -19.196 | 36.897 | 1.00 | 45.38 | BLGL |
| ATOM | 1298 | NZ  | LYS | 178 | -5.125 | -20.370 | 36.252 | 1.00 | 47.94 | BLGL |
| ATOM | 1299 | C   | LYS | 178 | -3.568 | -14.217 | 33.637 | 1.00 | 30.97 | BLGL |
| ATOM | 1300 | O   | LYS | 178 | -4.040 | -13.153 | 34.043 | 1.00 | 31.65 | BLGL |
| ATOM | 1301 | N   | MET | 179 | -2.333 | -14.306 | 33.149 | 1.00 | 29.06 | BLGL |
| ATOM | 1302 | CA  | MET | 179 | -1.485 | -13.126 | 33.062 | 1.00 | 26.50 | BLGL |
| ATOM | 1303 | CB  | MET | 179 | -0.110 | -13.481 | 32.521 | 1.00 | 27.08 | BLGL |
| ATOM | 1304 | CG  | MET | 179 | 0.789  | -14.179 | 33.507 | 1.00 | 29.22 | BLGL |
| ATOM | 1305 | SD  | MET | 179 | 2.433  | -14.378 | 32.801 | 1.00 | 32.04 | BLGL |
| ATOM | 1306 | CE  | MET | 179 | 2.432  | -16.100 | 32.529 | 1.00 | 37.19 | BLGL |
| ATOM | 1307 | C   | MET | 179 | -2.122 | -12.106 | 32.141 | 1.00 | 25.11 | BLGL |
| ATOM | 1308 | O   | MET | 179 | -2.206 | -10.924 | 32.478 | 1.00 | 24.38 | BLGL |
| ATOM | 1309 | N   | SER | 180 | -2.566 | -12.572 | 30.977 | 1.00 | 23.38 | BLGL |
| ATOM | 1310 | CA  | SER | 180 | -3.199 | -11.707 | 29.985 | 1.00 | 23.70 | BLGL |
| ATOM | 1311 | CB  | SER | 180 | -3.725 | -12.533 | 28.812 | 1.00 | 23.12 | BLGL |
| ATOM | 1312 | OG  | SER | 180 | -2.691 | -13.297 | 28.223 | 1.00 | 23.86 | BLGL |
| ATOM | 1313 | C   | SER | 180 | -4.348 | -10.933 | 30.605 | 1.00 | 24.08 | BLGL |
| ATOM | 1314 | O   | SER | 180 | -4.552 | -9.756  | 30.313 | 1.00 | 23.86 | BLGL |
| ATOM | 1315 | N   | GLN | 181 | -5.101 | -11.601 | 31.467 | 1.00 | 25.04 | BLGL |
| ATOM | 1316 | CA  | GLN | 181 | -6.226 | -10.965 | 32.129 | 1.00 | 27.04 | BLGL |
| ATOM | 1317 | CB  | GLN | 181 | -7.064 | -12.009 | 32.864 | 1.00 | 29.17 | BLGL |
| ATOM | 1318 | CG  | GLN | 181 | -7.820 | -12.940 | 31.932 | 1.00 | 33.08 | BLGL |
| ATOM | 1319 | CD  | GLN | 181 | -8.761 | -13.860 | 32.675 | 1.00 | 35.97 | BLGL |

# Fig. 4 cont.

| ATOM | 1320 | OE1 | GLN | 181 | -8.558 | -15.077 | 32.724 | 1.00 | 36.76 | BLGL |
|------|------|-----|-----|-----|--------|---------|--------|------|-------|------|
| ATOM | 1321 | NE2 | GLN | 181 | -9.801 | -13.280 | 33.269 | 1.00 | 37.03 | BLGL |
| ATOM | 1322 | C | GLN | 181 | -5.774 | -9.874 | 33.091 | 1.00 | 27.11 | BLGL |
| ATOM | 1323 | O | GLN | 181 | -6.459 | -8.864 | 33.252 | 1.00 | 28.46 | BLGL |
| ATOM | 1324 | N | LEU | 182 | -4.628 | -10.080 | 33.737 | 1.00 | 26.80 | BLGL |
| ATOM | 1325 | CA | LEU | 182 | -4.086 | -9.081 | 34.655 | 1.00 | 25.48 | BLGL |
| ATOM | 1326 | CB | LEU | 182 | -2.932 | -9.665 | 35.472 | 1.00 | 25.40 | BLGL |
| ATOM | 1327 | CG | LEU | 182 | -3.296 | -10.736 | 36.504 | 1.00 | 27.62 | BLGL |
| ATOM | 1328 | CD1 | LEU | 182 | -2.035 | -11.268 | 37.156 | 1.00 | 27.60 | BLGL |
| ATOM | 1329 | CD2 | LEU | 182 | -4.229 | -10.149 | 37.556 | 1.00 | 26.92 | BLGL |
| ATOM | 1330 | C | LEU | 182 | -3.591 | -7.899 | 33.823 | 1.00 | 24.10 | BLGL |
| ATOM | 1331 | O | LEU | 182 | -3.739 | -6.740 | 34.211 | 1.00 | 23.49 | BLGL |
| ATOM | 1332 | N | PHE | 183 | -3.000 | -8.211 | 32.675 | 1.00 | 21.91 | BLGL |
| ATOM | 1333 | CA | PHE | 183 | -2.512 | -7.187 | 31.770 | 1.00 | 22.28 | BLGL |
| ATOM | 1334 | CB | PHE | 183 | -1.888 | -7.826 | 30.528 | 1.00 | 21.38 | BLGL |
| ATOM | 1335 | CG | PHE | 183 | -0.500 | -8.347 | 30.737 | 1.00 | 20.19 | BLGL |
| ATOM | 1336 | CD1 | PHE | 183 | -0.064 | -9.469 | 30.042 | 1.00 | 20.38 | BLGL |
| ATOM | 1337 | CD2 | PHE | 183 | 0.385 | -7.704 | 31.597 | 1.00 | 22.77 | BLGL |
| ATOM | 1338 | CE1 | PHE | 183 | 1.236 | -9.953 | 30.192 | 1.00 | 20.30 | BLGL |
| ATOM | 1339 | CE2 | PHE | 183 | 1.693 | -8.174 | 31.761 | 1.00 | 24.59 | BLGL |
| ATOM | 1340 | CZ | PHE | 183 | 2.120 | -9.305 | 31.054 | 1.00 | 23.28 | BLGL |
| ATOM | 1341 | C | PHE | 183 | -3.668 | -6.283 | 31.348 | 1.00 | 22.44 | BLGL |
| ATOM | 1342 | O | PHE | 183 | -3.548 | -5.059 | 31.384 | 1.00 | 22.23 | BLGL |
| ATOM | 1343 | N | ASN | 184 | -4.792 | -6.881 | 30.954 | 1.00 | 22.00 | BLGL |
| ATOM | 1344 | CA | ASN | 184 | -5.939 | -6.087 | 30.533 | 1.00 | 20.53 | BLGL |
| ATOM | 1345 | CB | ASN | 184 | -7.012 | -6.964 | 29.895 | 1.00 | 20.92 | BLGL |
| ATOM | 1346 | CG | ASN | 184 | -6.677 | -7.345 | 28.474 | 1.00 | 21.95 | BLGL |
| ATOM | 1347 | OD1 | ASN | 184 | -6.162 | -6.535 | 27.708 | 1.00 | 24.93 | BLGL |
| ATOM | 1348 | ND2 | ASN | 184 | -6.983 | -8.579 | 28.108 | 1.00 | 26.02 | BLGL |
| ATOM | 1349 | C | ASN | 184 | -6.538 | -5.293 | 31.679 | 1.00 | 17.99 | BLGL |
| ATOM | 1350 | O | ASN | 184 | -7.053 | -4.199 | 31.474 | 1.00 | 18.30 | BLGL |
| ATOM | 1351 | N | ALA | 185 | -6.458 | -5.841 | 32.884 | 1.00 | 16.83 | BLGL |
| ATOM | 1352 | CA | ALA | 185 | -6.976 | -5.163 | 34.066 | 1.00 | 18.27 | BLGL |
| ATOM | 1353 | CB | ALA | 185 | -6.815 | -6.048 | 35.294 | 1.00 | 16.14 | BLGL |
| ATOM | 1354 | C | ALA | 185 | -6.215 | -3.857 | 34.261 | 1.00 | 18.87 | BLGL |
| ATOM | 1355 | O | ALA | 185 | -6.812 | -2.795 | 34.422 | 1.00 | 17.89 | BLGL |
| ATOM | 1356 | N | GLY | 186 | -4.888 | -3.945 | 34.244 | 1.00 | 20.07 | BLGL |
| ATOM | 1357 | CA | GLY | 186 | -4.073 | -2.756 | 34.409 | 1.00 | 19.75 | BLGL |
| ATOM | 1358 | C | GLY | 186 | -4.273 | -1.834 | 33.226 | 1.00 | 19.07 | BLGL |
| ATOM | 1359 | O | GLY | 186 | -4.367 | -0.620 | 33.373 | 1.00 | 20.22 | BLGL |
| ATOM | 1360 | N | SER | 187 | -4.345 | -2.424 | 32.042 | 1.00 | 18.72 | BLGL |
| ATOM | 1361 | CA | SER | 187 | -4.534 | -1.664 | 30.819 | 1.00 | 18.78 | BLGL |
| ATOM | 1362 | CB | SER | 187 | -4.570 | -2.618 | 29.627 | 1.00 | 19.99 | BLGL |
| ATOM | 1363 | OG | SER | 187 | -4.606 | -1.903 | 28.409 | 1.00 | 22.89 | BLGL |
| ATOM | 1364 | C | SER | 187 | -5.840 | -0.877 | 30.897 | 1.00 | 20.30 | BLGL |
| ATOM | 1365 | O | SER | 187 | -5.879 | 0.311 | 30.582 | 1.00 | 20.23 | BLGL |
| ATOM | 1366 | N | GLN | 188 | -6.903 | -1.554 | 31.325 | 1.00 | 19.43 | BLGL |
| ATOM | 1367 | CA | GLN | 188 | -8.233 | -0.960 | 31.465 | 1.00 | 20.10 | BLGL |
| ATOM | 1368 | CB | GLN | 188 | -9.192 | -1.990 | 32.093 | 1.00 | 21.27 | BLGL |
| ATOM | 1369 | CG | GLN | 188 | -10.592 | -1.480 | 32.439 | 1.00 | 24.00 | BLGL |
| ATOM | 1370 | CD | GLN | 188 | -11.358 | -0.973 | 31.228 | 1.00 | 29.54 | BLGL |
| ATOM | 1371 | OE1 | GLN | 188 | -11.546 | -1.695 | 30.242 | 1.00 | 33.67 | BLGL |
| ATOM | 1372 | NE2 | GLN | 188 | -11.808 | 0.274 | 31.295 | 1.00 | 28.21 | BLGL |
| ATOM | 1373 | C | GLN | 188 | -8.191 | 0.303 | 32.322 | 1.00 | 20.12 | BLGL |
| ATOM | 1374 | O | GLN | 188 | -8.779 | 1.322 | 31.984 | 1.00 | 19.92 | BLGL |
| ATOM | 1375 | N | ALA | 189 | -7.493 | 0.227 | 33.442 | 1.00 | 20.06 | BLGL |
| ATOM | 1376 | CA | ALA | 189 | -7.383 | 1.366 | 34.329 | 1.00 | 19.56 | BLGL |
| ATOM | 1377 | CB | ALA | 189 | -6.587 | 0.982 | 35.563 | 1.00 | 18.86 | BLGL |
| ATOM | 1378 | C | ALA | 189 | -6.728 | 2.546 | 33.626 | 1.00 | 19.66 | BLGL |
| ATOM | 1379 | O | ALA | 189 | -7.150 | 3.681 | 33.805 | 1.00 | 20.48 | BLGL |
| ATOM | 1380 | N | VAL | 190 | -5.697 | 2.273 | 32.831 | 1.00 | 19.85 | BLGL |
| ATOM | 1381 | CA | VAL | 190 | -4.984 | 3.324 | 32.108 | 1.00 | 21.68 | BLGL |
| ATOM | 1382 | CB | VAL | 190 | -3.717 | 2.755 | 31.378 | 1.00 | 21.13 | BLGL |
| ATOM | 1383 | CG1 | VAL | 190 | -2.955 | 3.875 | 30.675 | 1.00 | 17.97 | BLGL |
| ATOM | 1384 | CG2 | VAL | 190 | -2.809 | 2.069 | 32.376 | 1.00 | 18.02 | BLGL |
| ATOM | 1385 | C | VAL | 190 | -5.922 | 3.966 | 31.087 | 1.00 | 22.56 | BLGL |

# Fig. 4 cont.

| ATOM | 1386 | O | VAL | 190 | -6.041 | 5.190 | 31.007 | 1.00 | 21.59 | BLGL |
|------|------|------|-----|-----|--------|-------|--------|------|-------|------|
| ATOM | 1387 | N | ARG | 191 | -6.590 | 3.122 | 30.311 | 1.00 | 24.93 | BLGL |
| ATOM | 1388 | CA | ARG | 191 | -7.528 | 3.577 | 29.297 | 1.00 | 24.90 | BLGL |
| ATOM | 1389 | CB | ARG | 191 | -8.199 | 2.375 | 28.640 | 1.00 | 22.96 | BLGL |
| ATOM | 1390 | CG | ARG | 191 | -7.687 | 2.059 | 27.236 | 1.00 | 25.30 | BLGL |
| ATOM | 1391 | CD | ARG | 191 | -6.416 | 1.230 | 27.171 | 1.00 | 24.11 | BLGL |
| ATOM | 1392 | NE | ARG | 191 | -5.369 | 1.936 | 26.503 | 1.00 | 24.46 | BLGL |
| ATOM | 1393 | CZ | ARG | 191 | -4.581 | 1.653 | 25.474 | 1.00 | 21.34 | BLGL |
| ATOM | 1394 | NH1 | ARG | 191 | -3.733 | 2.613 | 25.208 | 1.00 | 22.37 | BLGL |
| ATOM | 1395 | NH2 | ARG | 191 | -4.584 | 0.551 | 24.731 | 1.00 | 21.45 | BLGL |
| ATOM | 1396 | C | ARG | 191 | -8.590 | 4.492 | 29.892 | 1.00 | 25.14 | BLGL |
| ATOM | 1397 | O | ARG | 191 | -8.904 | 5.535 | 29.334 | 1.00 | 27.85 | BLGL |
| ATOM | 1398 | N | GLU | 192 | -9.145 | 4.098 | 31.026 | 1.00 | 25.90 | BLGL |
| ATOM | 1399 | CA | GLU | 192 | -10.170 | 4.895 | 31.683 | 1.00 | 28.14 | BLGL |
| ATOM | 1400 | CB | GLU | 192 | -10.761 | 4.129 | 32.865 | 1.00 | 28.90 | BLGL |
| ATOM | 1401 | CG | GLU | 192 | -11.776 | 3.079 | 32.494 | 1.00 | 31.91 | BLGL |
| ATOM | 1402 | CD | GLU | 192 | -12.200 | 2.266 | 33.697 | 1.00 | 32.43 | BLGL |
| ATOM | 1403 | OE1 | GLU | 192 | -12.359 | 2.874 | 34.772 | 1.00 | 28.80 | BLGL |
| ATOM | 1404 | OE2 | GLU | 192 | -12.378 | 1.033 | 33.569 | 1.00 | 34.08 | BLGL |
| ATOM | 1405 | C | GLU | 192 | -9.630 | 6.223 | 32.190 | 1.00 | 28.73 | BLGL |
| ATOM | 1406 | O | GLU | 192 | -10.352 | 7.219 | 32.278 | 1.00 | 31.92 | BLGL |
| ATOM | 1407 | N | THR | 193 | -8.355 | 6.237 | 32.541 | 1.00 | 27.87 | BLGL |
| ATOM | 1408 | CA | THR | 193 | -7.741 | 7.445 | 33.064 | 1.00 | 26.29 | BLGL |
| ATOM | 1409 | CB | THR | 193 | -6.416 | 7.098 | 33.780 | 1.00 | 25.98 | BLGL |
| ATOM | 1410 | OG1 | THR | 193 | -6.697 | 6.231 | 34.884 | 1.00 | 27.07 | BLGL |
| ATOM | 1411 | CG2 | THR | 193 | -5.725 | 8.350 | 34.296 | 1.00 | 24.23 | BLGL |
| ATOM | 1412 | C | THR | 193 | -7.488 | 8.500 | 31.990 | 1.00 | 25.40 | BLGL |
| ATOM | 1413 | O | THR | 193 | -7.827 | 9.666 | 32.160 | 1.00 | 22.00 | BLGL |
| ATOM | 1414 | N | ASP | 194 | -6.909 | 8.084 | 30.872 | 1.00 | 27.05 | BLGL |
| ATOM | 1415 | CA | ASP | 194 | -6.585 | 9.020 | 29.810 | 1.00 | 27.87 | BLGL |
| ATOM | 1416 | CB | ASP | 194 | -5.396 | 9.870 | 30.271 | 1.00 | 29.53 | BLGL |
| ATOM | 1417 | CG | ASP | 194 | -4.956 | 10.881 | 29.243 | 1.00 | 32.75 | BLGL |
| ATOM | 1418 | OD1 | ASP | 194 | -4.131 | 11.746 | 29.606 | 1.00 | 34.57 | BLGL |
| ATOM | 1419 | OD2 | ASP | 194 | -5.418 | 10.816 | 28.081 | 1.00 | 35.03 | BLGL |
| ATOM | 1420 | C | ASP | 194 | -6.245 | 8.249 | 28.546 | 1.00 | 27.55 | BLGL |
| ATOM | 1421 | O | ASP | 194 | -5.389 | 7.368 | 28.565 | 1.00 | 29.57 | BLGL |
| ATOM | 1422 | N | SER | 195 | -6.917 | 8.580 | 27.449 | 1.00 | 27.67 | BLGL |
| ATOM | 1423 | CA | SER | 195 | -6.690 | 7.903 | 26.169 | 1.00 | 30.14 | BLGL |
| ATOM | 1424 | CB | SER | 195 | -7.748 | 8.333 | 25.154 | 1.00 | 31.04 | BLGL |
| ATOM | 1425 | OG | SER | 195 | -9.041 | 7.986 | 25.608 | 1.00 | 38.90 | BLGL |
| ATOM | 1426 | C | SER | 195 | -5.314 | 8.137 | 25.553 | 1.00 | 29.28 | BLGL |
| ATOM | 1427 | O | SER | 195 | -4.830 | 7.319 | 24.773 | 1.00 | 26.29 | BLGL |
| ATOM | 1428 | N | ASN | 196 | -4.690 | 9.255 | 25.903 | 1.00 | 30.46 | BLGL |
| ATOM | 1429 | CA | ASN | 196 | -3.387 | 9.600 | 25.358 | 1.00 | 32.52 | BLGL |
| ATOM | 1430 | CB | ASN | 196 | -3.147 | 11.097 | 25.514 | 1.00 | 38.65 | BLGL |
| ATOM | 1431 | CG | ASN | 196 | -4.246 | 11.919 | 24.892 | 1.00 | 45.74 | BLGL |
| ATOM | 1432 | OD1 | ASN | 196 | -4.436 | 11.902 | 23.672 | 1.00 | 47.81 | BLGL |
| ATOM | 1433 | ND2 | ASN | 196 | -4.996 | 12.637 | 25.729 | 1.00 | 49.19 | BLGL |
| ATOM | 1434 | C | ASN | 196 | -2.232 | 8.838 | 25.981 | 1.00 | 30.86 | BLGL |
| ATOM | 1435 | O | ASN | 196 | -1.141 | 8.779 | 25.411 | 1.00 | 31.65 | BLGL |
| ATOM | 1436 | N | ILE | 197 | -2.459 | 8.260 | 27.153 | 1.00 | 28.33 | BLGL |
| ATOM | 1437 | CA | ILE | 197 | -1.403 | 7.517 | 27.816 | 1.00 | 25.33 | BLGL |
| ATOM | 1438 | CB | ILE | 197 | -1.771 | 7.224 | 29.282 | 1.00 | 24.62 | BLGL |
| ATOM | 1439 | CG2 | ILE | 197 | -0.720 | 6.335 | 29.919 | 1.00 | 24.24 | BLGL |
| ATOM | 1440 | CG1 | ILE | 197 | -1.873 | 8.542 | 30.053 | 1.00 | 24.08 | BLGL |
| ATOM | 1441 | CD1 | ILE | 197 | -2.239 | 8.380 | 31.513 | 1.00 | 24.86 | BLGL |
| ATOM | 1442 | C | ILE | 197 | -1.149 | 6.222 | 27.064 | 1.00 | 23.64 | BLGL |
| ATOM | 1443 | O | ILE | 197 | -2.081 | 5.487 | 26.748 | 1.00 | 23.83 | BLGL |
| ATOM | 1444 | N | LEU | 198 | 0.116 | 5.962 | 26.754 | 1.00 | 21.57 | BLGL |
| ATOM | 1445 | CA | LEU | 198 | 0.483 | 4.751 | 26.039 | 1.00 | 21.61 | BLGL |
| ATOM | 1446 | CB | LEU | 198 | 1.787 | 4.962 | 25.271 | 1.00 | 21.02 | BLGL |
| ATOM | 1447 | CG | LEU | 198 | 1.683 | 5.885 | 24.055 | 1.00 | 22.44 | BLGL |
| ATOM | 1448 | CD1 | LEU | 198 | 3.062 | 6.252 | 23.554 | 1.00 | 22.29 | BLGL |
| ATOM | 1449 | CD2 | LEU | 198 | 0.881 | 5.188 | 22.967 | 1.00 | 23.53 | BLGL |
| ATOM | 1450 | C | LEU | 198 | 0.653 | 3.605 | 27.013 | 1.00 | 21.75 | BLGL |
| ATOM | 1451 | O | LEU | 198 | 1.250 | 3.776 | 28.073 | 1.00 | 23.44 | BLGL |

**Fig. 4 cont.**

| ATOM | 1452 | N   | VAL | 199 | 0.114  | 2.441   | 26.666 | 1.00 20.49 | BLGL |
|------|------|-----|-----|-----|--------|---------|--------|------------|------|
| ATOM | 1453 | CA  | VAL | 199 | 0.244  | 1.266   | 27.516 | 1.00 19.26 | BLGL |
| ATOM | 1454 | CB  | VAL | 199 | -1.040 | 0.450   | 27.555 | 1.00 19.98 | BLGL |
| ATOM | 1455 | CG1 | VAL | 199 | -0.816 | -0.815  | 28.364 | 1.00 19.20 | BLGL |
| ATOM | 1456 | CG2 | VAL | 199 | -2.148 | 1.282   | 28.149 | 1.00 21.20 | BLGL |
| ATOM | 1457 | C   | VAL | 199 | 1.352  | 0.376   | 26.979 | 1.00 18.65 | BLGL |
| ATOM | 1458 | O   | VAL | 199 | 1.329  | -0.029  | 25.818 | 1.00 16.57 | BLGL |
| ATOM | 1459 | N   | ALA | 200 | 2.314  | 0.061   | 27.839 | 1.00 17.36 | BLGL |
| ATOM | 1460 | CA  | ALA | 200 | 3.436  | -0.760  | 27.432 | 1.00 17.13 | BLGL |
| ATOM | 1461 | CB  | ALA | 200 | 4.701  | 0.087   | 27.427 | 1.00 15.68 | BLGL |
| ATOM | 1462 | C   | ALA | 200 | 3.645  | -1.991  | 28.299 | 1.00 16.72 | BLGL |
| ATOM | 1463 | O   | ALA | 200 | 3.403  | -1.960  | 29.501 | 1.00 15.94 | BLGL |
| ATOM | 1464 | N   | LEU | 201 | 4.079  | -3.077  | 27.661 | 1.00 17.11 | BLGL |
| ATOM | 1465 | CA  | LEU | 201 | 4.390  | -4.332  | 28.339 | 1.00 17.16 | BLGL |
| ATOM | 1466 | CB  | LEU | 201 | 3.638  | -5.502  | 27.706 | 1.00 17.16 | BLGL |
| ATOM | 1467 | CG  | LEU | 201 | 2.114  | -5.388  | 27.753 | 1.00 17.50 | BLGL |
| ATOM | 1468 | CD1 | LEU | 201 | 1.497  | -6.671  | 27.236 | 1.00 20.85 | BLGL |
| ATOM | 1469 | CD2 | LEU | 201 | 1.654  | -5.132  | 29.172 | 1.00 19.12 | BLGL |
| ATOM | 1470 | C   | LEU | 201 | 5.907  | -4.497  | 28.186 | 1.00 17.78 | BLGL |
| ATOM | 1471 | O   | LEU | 201 | 6.465  | -4.279  | 27.111 | 1.00 17.49 | BLGL |
| ATOM | 1472 | N   | HIS | 202 | 6.568  | -4.874  | 29.272 | 1.00 18.05 | BLGL |
| ATOM | 1473 | CA  | HIS | 202 | 8.018  | -4.981  | 29.294 | 1.00 17.54 | BLGL |
| ATOM | 1474 | CB  | HIS | 202 | 8.519  | -4.129  | 30.460 | 1.00 17.68 | BLGL |
| ATOM | 1475 | CG  | HIS | 202 | 10.002 | -4.110  | 30.616 | 1.00 19.94 | BLGL |
| ATOM | 1476 | CD2 | HIS | 202 | 10.998 | -4.372  | 29.741 | 1.00 20.39 | BLGL |
| ATOM | 1477 | ND1 | HIS | 202 | 10.613 | -3.773  | 31.805 | 1.00 21.65 | BLGL |
| ATOM | 1478 | CE1 | HIS | 202 | 11.922 | -3.831  | 31.655 | 1.00 22.99 | BLGL |
| ATOM | 1479 | NE2 | HIS | 202 | 12.183 | -4.193  | 30.411 | 1.00 23.44 | BLGL |
| ATOM | 1480 | C   | HIS | 202 | 8.569  | -6.400  | 29.402 | 1.00 18.30 | BLGL |
| ATOM | 1481 | O   | HIS | 202 | 8.272  | -7.122  | 30.354 | 1.00 18.51 | BLGL |
| ATOM | 1482 | N   | PHE | 203 | 9.386  | -6.790  | 28.429 | 1.00 16.01 | BLGL |
| ATOM | 1483 | CA  | PHE | 203 | 9.989  | -8.114  | 28.431 | 1.00 16.62 | BLGL |
| ATOM | 1484 | CB  | PHE | 203 | 9.398  | -8.963  | 27.316 | 1.00 13.11 | BLGL |
| ATOM | 1485 | CG  | PHE | 203 | 7.912  | -9.055  | 27.375 | 1.00 17.34 | BLGL |
| ATOM | 1486 | CD1 | PHE | 203 | 7.116  | -8.119  | 26.724 | 1.00 17.15 | BLGL |
| ATOM | 1487 | CD2 | PHE | 203 | 7.299  | -10.037 | 28.144 | 1.00 15.95 | BLGL |
| ATOM | 1488 | CE1 | PHE | 203 | 5.738  | -8.158  | 26.840 | 1.00 16.32 | BLGL |
| ATOM | 1489 | CE2 | PHE | 203 | 5.925  | -10.083 | 28.266 | 1.00 16.04 | BLGL |
| ATOM | 1490 | CZ  | PHE | 203 | 5.141  | -9.140  | 27.612 | 1.00 18.54 | BLGL |
| ATOM | 1491 | C   | PHE | 203 | 11.504 | -8.033  | 28.274 | 1.00 19.65 | BLGL |
| ATOM | 1492 | O   | PHE | 203 | 12.051 | -6.987  | 27.910 | 1.00 21.99 | BLGL |
| ATOM | 1493 | N   | THR | 204 | 12.188 | -9.135  | 28.552 | 1.00 17.81 | BLGL |
| ATOM | 1494 | CA  | THR | 204 | 13.634 | -9.133  | 28.426 | 1.00 18.21 | BLGL |
| ATOM | 1495 | CB  | THR | 204 | 14.314 | -8.849  | 29.798 | 1.00 17.19 | BLGL |
| ATOM | 1496 | OG1 | THR | 204 | 15.726 | -8.736  | 29.611 | 1.00 14.37 | BLGL |
| ATOM | 1497 | CG2 | THR | 204 | 14.006 | -9.951  | 30.809 | 1.00 13.65 | BLGL |
| ATOM | 1498 | C   | THR | 204 | 14.161 | -10.428 | 27.809 | 1.00 18.61 | BLGL |
| ATOM | 1499 | O   | THR | 204 | 13.394 | -11.352 | 27.534 | 1.00 16.21 | BLGL |
| ATOM | 1500 | N   | ASN | 205 | 15.469 | -10.473 | 27.580 | 1.00 17.26 | BLGL |
| ATOM | 1501 | CA  | ASN | 205 | 16.112 | -11.622 | 26.964 | 1.00 17.80 | BLGL |
| ATOM | 1502 | CB  | ASN | 205 | 15.814 | -12.907 | 27.728 | 1.00 18.45 | BLGL |
| ATOM | 1503 | CG  | ASN | 205 | 16.601 | -13.000 | 29.001 | 1.00 18.12 | BLGL |
| ATOM | 1504 | OD1 | ASN | 205 | 16.070 | -12.811 | 30.094 | 1.00 20.78 | BLGL |
| ATOM | 1505 | ND2 | ASN | 205 | 17.890 | -13.266 | 28.868 | 1.00 18.03 | BLGL |
| ATOM | 1506 | C   | ASN | 205 | 15.701 | -11.784 | 25.520 | 1.00 17.89 | BLGL |
| ATOM | 1507 | O   | ASN | 205 | 15.129 | -12.800 | 25.135 | 1.00 18.21 | BLGL |
| ATOM | 1508 | N   | PRO | 206 | 15.988 | -10.771 | 24.697 | 1.00 18.39 | BLGL |
| ATOM | 1509 | CD  | PRO | 206 | 16.580 | -9.480  | 25.080 | 1.00 15.66 | BLGL |
| ATOM | 1510 | CA  | PRO | 206 | 15.657 | -10.778 | 23.273 | 1.00 19.70 | BLGL |
| ATOM | 1511 | CB  | PRO | 206 | 15.903 | -9.334  | 22.867 | 1.00 19.33 | BLGL |
| ATOM | 1512 | CG  | PRO | 206 | 17.029 | -8.939  | 23.756 | 1.00 16.74 | BLGL |
| ATOM | 1513 | C   | PRO | 206 | 16.500 | -11.748 | 22.459 | 1.00 21.36 | BLGL |
| ATOM | 1514 | O   | PRO | 206 | 16.158 | -12.055 | 21.318 | 1.00 22.70 | BLGL |
| ATOM | 1515 | N   | GLU | 207 | 17.601 | -12.224 | 23.034 | 1.00 23.27 | BLGL |
| ATOM | 1516 | CA  | GLU | 207 | 18.478 | -13.154 | 22.324 | 1.00 25.47 | BLGL |
| ATOM | 1517 | CB  | GLU | 207 | 19.871 | -13.210 | 22.959 | 1.00 26.18 | BLGL |

# Fig. 4 cont.

| ATOM | 1518 | CG | GLU | 207 | 20.021 | -12.502 | 24.288 | 1.00 | 30.25 | BLGL |
|------|------|-----|-----|-----|--------|---------|--------|------|-------|------|
| ATOM | 1519 | CD | GLU | 207 | 19.242 | -13.139 | 25.413 | 1.00 | 29.52 | BLGL |
| ATOM | 1520 | OE1 | GLU | 207 | 19.387 | -14.353 | 25.643 | 1.00 | 33.25 | BLGL |
| ATOM | 1521 | OE2 | GLU | 207 | 18.495 | -12.413 | 26.081 | 1.00 | 29.56 | BLGL |
| ATOM | 1522 | C | GLU | 207 | 17.924 | -14.561 | 22.258 | 1.00 | 26.20 | BLGL |
| ATOM | 1523 | O | GLU | 207 | 18.354 | -15.357 | 21.426 | 1.00 | 29.50 | BLGL |
| ATOM | 1524 | N | THR | 208 | 16.982 | -14.873 | 23.139 | 1.00 | 25.50 | BLGL |
| ATOM | 1525 | CA | THR | 208 | 16.384 | -16.196 | 23.151 | 1.00 | 25.38 | BLGL |
| ATOM | 1526 | CB | THR | 208 | 15.419 | -16.349 | 24.314 | 1.00 | 25.02 | BLGL |
| ATOM | 1527 | OG1 | THR | 208 | 16.108 | -16.063 | 25.532 | 1.00 | 24.40 | BLGL |
| ATOM | 1528 | CG2 | THR | 208 | 14.871 | -17.765 | 24.361 | 1.00 | 24.75 | BLGL |
| ATOM | 1529 | C | THR | 208 | 15.628 | -16.435 | 21.853 | 1.00 | 24.66 | BLGL |
| ATOM | 1530 | O | THR | 208 | 14.689 | -15.711 | 21.531 | 1.00 | 23.66 | BLGL |
| ATOM | 1531 | N | SER | 209 | 16.047 | -17.455 | 21.114 | 1.00 | 24.67 | BLGL |
| ATOM | 1532 | CA | SER | 209 | 15.424 | -17.791 | 19.842 | 1.00 | 25.56 | BLGL |
| ATOM | 1533 | CB | SER | 209 | 15.971 | -19.120 | 19.334 | 1.00 | 23.59 | BLGL |
| ATOM | 1534 | OG | SER | 209 | 15.290 | -19.524 | 18.166 | 1.00 | 26.21 | BLGL |
| ATOM | 1535 | C | SER | 209 | 13.896 | -17.862 | 19.885 | 1.00 | 26.32 | BLGL |
| ATOM | 1536 | O | SER | 209 | 13.321 | -18.668 | 20.632 | 1.00 | 23.52 | BLGL |
| ATOM | 1537 | N | GLY | 210 | 13.257 | -17.004 | 19.083 | 1.00 | 26.00 | BLGL |
| ATOM | 1538 | CA | GLY | 210 | 11.803 | -16.966 | 18.977 | 1.00 | 25.41 | BLGL |
| ATOM | 1539 | C | GLY | 210 | 10.990 | -16.593 | 20.204 | 1.00 | 26.60 | BLGL |
| ATOM | 1540 | O | GLY | 210 | 9.768 | -16.755 | 20.215 | 1.00 | 26.52 | BLGL |
| ATOM | 1541 | N | ARG | 211 | 11.659 | -16.080 | 21.231 | 1.00 | 27.83 | BLGL |
| ATOM | 1542 | CA | ARG | 211 | 11.004 | -15.692 | 22.478 | 1.00 | 25.31 | BLGL |
| ATOM | 1543 | CB | ARG | 211 | 12.046 | -15.244 | 23.496 | 1.00 | 26.05 | BLGL |
| ATOM | 1544 | CG | ARG | 211 | 11.487 | -15.024 | 24.881 | 1.00 | 26.98 | BLGL |
| ATOM | 1545 | CD | ARG | 211 | 12.479 | -14.289 | 25.747 | 1.00 | 28.49 | BLGL |
| ATOM | 1546 | NE | ARG | 211 | 12.362 | -14.719 | 27.125 | 1.00 | 32.45 | BLGL |
| ATOM | 1547 | CZ | ARG | 211 | 13.043 | -15.727 | 27.655 | 1.00 | 34.26 | BLGL |
| ATOM | 1548 | NH1 | ARG | 211 | 13.903 | -16.408 | 26.920 | 1.00 | 33.07 | BLGL |
| ATOM | 1549 | NH2 | ARG | 211 | 12.850 | -16.067 | 28.924 | 1.00 | 40.91 | BLGL |
| ATOM | 1550 | C | ARG | 211 | 9.977 | -14.580 | 22.294 | 1.00 | 24.24 | BLGL |
| ATOM | 1551 | O | ARG | 211 | 8.806 | -14.744 | 22.634 | 1.00 | 24.47 | BLGL |
| ATOM | 1552 | N | TYR | 212 | 10.413 | -13.440 | 21.768 | 1.00 | 22.57 | BLGL |
| ATOM | 1553 | CA | TYR | 212 | 9.499 | -12.323 | 21.558 | 1.00 | 20.27 | BLGL |
| ATOM | 1554 | CB | TYR | 212 | 10.262 | -11.080 | 21.093 | 1.00 | 18.26 | BLGL |
| ATOM | 1555 | CG | TYR | 212 | 11.063 | -10.409 | 22.188 | 1.00 | 20.40 | BLGL |
| ATOM | 1556 | CD1 | TYR | 212 | 11.669 | -9.170 | 21.972 | 1.00 | 19.09 | BLGL |
| ATOM | 1557 | CE1 | TYR | 212 | 12.387 | -8.538 | 22.982 | 1.00 | 16.98 | BLGL |
| ATOM | 1558 | CD2 | TYR | 212 | 11.204 | -11.001 | 23.445 | 1.00 | 17.87 | BLGL |
| ATOM | 1559 | CE2 | TYR | 212 | 11.919 | -10.377 | 24.457 | 1.00 | 15.68 | BLGL |
| ATOM | 1560 | CZ | TYR | 212 | 12.505 | -9.147 | 24.225 | 1.00 | 16.21 | BLGL |
| ATOM | 1561 | OH | TYR | 212 | 13.200 | -8.514 | 25.235 | 1.00 | 15.74 | BLGL |
| ATOM | 1562 | C | TYR | 212 | 8.398 | -12.670 | 20.559 | 1.00 | 20.87 | BLGL |
| ATOM | 1563 | O | TYR | 212 | 7.259 | -12.237 | 20.712 | 1.00 | 20.22 | BLGL |
| ATOM | 1564 | N | ALA | 213 | 8.734 | -13.449 | 19.537 | 1.00 | 19.68 | BLGL |
| ATOM | 1565 | CA | ALA | 213 | 7.742 | -13.847 | 18.547 | 1.00 | 19.79 | BLGL |
| ATOM | 1566 | CB | ALA | 213 | 8.399 | -14.687 | 17.454 | 1.00 | 17.89 | BLGL |
| ATOM | 1567 | C | ALA | 213 | 6.629 | -14.642 | 19.231 | 1.00 | 19.99 | BLGL |
| ATOM | 1568 | O | ALA | 213 | 5.451 | -14.479 | 18.911 | 1.00 | 19.71 | BLGL |
| ATOM | 1569 | N | TRP | 214 | 7.009 | -15.496 | 20.176 | 1.00 | 20.09 | BLGL |
| ATOM | 1570 | CA | TRP | 214 | 6.039 | -16.309 | 20.900 | 1.00 | 21.30 | BLGL |
| ATOM | 1571 | CB | TRP | 214 | 6.753 | -17.375 | 21.732 | 1.00 | 22.71 | BLGL |
| ATOM | 1572 | CG | TRP | 214 | 5.815 | -18.281 | 22.468 | 1.00 | 24.60 | BLGL |
| ATOM | 1573 | CD2 | TRP | 214 | 5.308 | -18.094 | 23.795 | 1.00 | 24.97 | BLGL |
| ATOM | 1574 | CE2 | TRP | 214 | 4.449 | -19.183 | 24.074 | 1.00 | 24.59 | BLGL |
| ATOM | 1575 | CE3 | TRP | 214 | 5.496 | -17.112 | 24.775 | 1.00 | 25.69 | BLGL |
| ATOM | 1576 | CD1 | TRP | 214 | 5.256 | -19.440 | 22.005 | 1.00 | 24.97 | BLGL |
| ATOM | 1577 | NE1 | TRP | 214 | 4.436 | -19.989 | 22.966 | 1.00 | 25.84 | BLGL |
| ATOM | 1578 | CZ2 | TRP | 214 | 3.780 | -19.319 | 25.294 | 1.00 | 22.78 | BLGL |
| ATOM | 1579 | CZ3 | TRP | 214 | 4.829 | -17.248 | 25.991 | 1.00 | 27.53 | BLGL |
| ATOM | 1580 | CH2 | TRP | 214 | 3.981 | -18.345 | 26.238 | 1.00 | 24.84 | BLGL |
| ATOM | 1581 | C | TRP | 214 | 5.167 | -15.453 | 21.816 | 1.00 | 21.83 | BLGL |
| ATOM | 1582 | O | TRP | 214 | 3.948 | -15.630 | 21.857 | 1.00 | 20.77 | BLGL |
| ATOM | 1583 | N | ILE | 215 | 5.793 | -14.531 | 22.550 | 1.00 | 21.49 | BLGL |

# Fig. 4 cont.

| ATOM | 1584 | CA | ILE | 215 | 5.067 | -13.654 | 23.469 | 1.00 | 19.18 | BLGL |
|------|------|-----|-----|-----|--------|---------|--------|------|-------|------|
| ATOM | 1585 | CB | ILE | 215 | 6.038 | -12.771 | 24.300 | 1.00 | 19.85 | BLGL |
| ATOM | 1586 | CG2 | ILE | 215 | 5.257 | -11.811 | 25.198 | 1.00 | 15.32 | BLGL |
| ATOM | 1587 | CG1 | ILE | 215 | 6.930 | -13.651 | 25.170 | 1.00 | 18.25 | BLGL |
| ATOM | 1588 | CD1 | ILE | 215 | 7.930 | -12.876 | 25.975 | 1.00 | 15.25 | BLGL |
| ATOM | 1589 | C | ILE | 215 | 4.104 | -12.740 | 22.725 | 1.00 | 19.79 | BLGL |
| ATOM | 1590 | O | ILE | 215 | 2.964 | -12.550 | 23.146 | 1.00 | 18.73 | BLGL |
| ATOM | 1591 | N | ALA | 216 | 4.565 | -12.163 | 21.621 | 1.00 | 19.35 | BLGL |
| ATOM | 1592 | CA | ALA | 216 | 3.723 | -11.275 | 20.840 | 1.00 | 18.57 | BLGL |
| ATOM | 1593 | CB | ALA | 216 | 4.492 | -10.751 | 19.650 | 1.00 | 18.16 | BLGL |
| ATOM | 1594 | C | ALA | 216 | 2.472 | -12.020 | 20.378 | 1.00 | 20.55 | BLGL |
| ATOM | 1595 | O | ALA | 216 | 1.359 | -11.501 | 20.466 | 1.00 | 16.58 | BLGL |
| ATOM | 1596 | N | GLU | 217 | 2.669 | -13.242 | 19.890 | 1.00 | 22.90 | BLGL |
| ATOM | 1597 | CA | GLU | 217 | 1.569 | -14.077 | 19.419 | 1.00 | 24.77 | BLGL |
| ATOM | 1598 | CB | GLU | 217 | 2.122 | -15.338 | 18.747 | 1.00 | 28.27 | BLGL |
| ATOM | 1599 | CG | GLU | 217 | 1.063 | -16.371 | 18.379 | 1.00 | 33.34 | BLGL |
| ATOM | 1600 | CD | GLU | 217 | -0.002 | -15.823 | 17.449 | 1.00 | 35.08 | BLGL |
| ATOM | 1601 | OE1 | GLU | 217 | -1.049 | -16.485 | 17.288 | 1.00 | 39.18 | BLGL |
| ATOM | 1602 | OE2 | GLU | 217 | 0.208 | -14.737 | 16.875 | 1.00 | 35.59 | BLGL |
| ATOM | 1603 | C | GLU | 217 | 0.623 | -14.468 | 20.560 | 1.00 | 24.16 | BLGL |
| ATOM | 1604 | O | GLU | 217 | -0.596 | -14.464 | 20.395 | 1.00 | 22.67 | BLGL |
| ATOM | 1605 | N | THR | 218 | 1.195 | -14.805 | 21.713 | 1.00 | 24.08 | BLGL |
| ATOM | 1606 | CA | THR | 218 | 0.412 | -15.191 | 22.878 | 1.00 | 23.79 | BLGL |
| ATOM | 1607 | CB | THR | 218 | 1.334 | -15.684 | 24.027 | 1.00 | 25.12 | BLGL |
| ATOM | 1608 | OG1 | THR | 218 | 1.985 | -16.896 | 23.630 | 1.00 | 26.14 | BLGL |
| ATOM | 1609 | CG2 | THR | 218 | 0.537 | -15.942 | 25.298 | 1.00 | 23.98 | BLGL |
| ATOM | 1610 | C | THR | 218 | -0.429 | -14.014 | 23.362 | 1.00 | 22.94 | BLGL |
| ATOM | 1611 | O | THR | 218 | -1.600 | -14.179 | 23.692 | 1.00 | 24.35 | BLGL |
| ATOM | 1612 | N | LEU | 219 | 0.160 | -12.825 | 23.401 | 1.00 | 21.92 | BLGL |
| ATOM | 1613 | CA | LEU | 219 | -0.578 | -11.644 | 23.846 | 1.00 | 23.28 | BLGL |
| ATOM | 1614 | CB | LEU | 219 | 0.333 | -10.410 | 23.863 | 1.00 | 21.92 | BLGL |
| ATOM | 1615 | CG | LEU | 219 | 1.462 | -10.359 | 24.893 | 1.00 | 18.90 | BLGL |
| ATOM | 1616 | CD1 | LEU | 219 | 2.386 | -9.209 | 24.570 | 1.00 | 14.80 | BLGL |
| ATOM | 1617 | CD2 | LEU | 219 | 0.879 | -10.220 | 26.289 | 1.00 | 16.33 | BLGL |
| ATOM | 1618 | C | LEU | 219 | -1.753 | -11.394 | 22.903 | 1.00 | 24.55 | BLGL |
| ATOM | 1619 | O | LEU | 219 | -2.850 | -11.031 | 23.322 | 1.00 | 25.23 | BLGL |
| ATOM | 1620 | N | HIS | 220 | -1.512 | -11.603 | 21.619 | 1.00 | 25.34 | BLGL |
| ATOM | 1621 | CA | HIS | 220 | -2.539 | -11.401 | 20.622 | 1.00 | 25.88 | BLGL |
| ATOM | 1622 | CB | HIS | 220 | -1.904 | -11.450 | 19.236 | 1.00 | 27.15 | BLGL |
| ATOM | 1623 | CG | HIS | 220 | -2.888 | -11.366 | 18.116 | 1.00 | 31.81 | BLGL |
| ATOM | 1624 | CD2 | HIS | 220 | -3.485 | -10.300 | 17.529 | 1.00 | 31.02 | BLGL |
| ATOM | 1625 | ND1 | HIS | 220 | -3.388 | -12.486 | 17.483 | 1.00 | 33.38 | BLGL |
| ATOM | 1626 | CE1 | HIS | 220 | -4.250 | -12.111 | 16.554 | 1.00 | 33.29 | BLGL |
| ATOM | 1627 | NE2 | HIS | 220 | -4.326 | -10.791 | 16.562 | 1.00 | 32.86 | BLGL |
| ATOM | 1628 | C | HIS | 220 | -3.665 | -12.423 | 20.743 | 1.00 | 26.70 | BLGL |
| ATOM | 1629 | O | HIS | 220 | -4.839 | -12.076 | 20.617 | 1.00 | 25.81 | BLGL |
| ATOM | 1630 | N | ARG | 221 | -3.312 | -13.679 | 20.993 | 1.00 | 28.18 | BLGL |
| ATOM | 1631 | CA | ARG | 221 | -4.314 | -14.730 | 21.133 | 1.00 | 30.04 | BLGL |
| ATOM | 1632 | CB | ARG | 221 | -3.648 | -16.090 | 21.361 | 1.00 | 33.95 | BLGL |
| ATOM | 1633 | CG | ARG | 221 | -3.038 | -16.680 | 20.095 | 1.00 | 40.22 | BLGL |
| ATOM | 1634 | CD | ARG | 221 | -2.052 | -17.802 | 20.368 | 1.00 | 47.28 | BLGL |
| ATOM | 1635 | NE | ARG | 221 | -2.419 | -19.012 | 19.696 | 1.00 | 52.72 | BLGL |
| ATOM | 1636 | CZ | ARG | 221 | -1.881 | -19.711 | 18.699 | 1.00 | 54.00 | BLGL |
| ATOM | 1637 | NH1 | ARG | 221 | -2.572 | -20.786 | 18.387 | 1.00 | 56.27 | BLGL |
| ATOM | 1638 | NH2 | ARG | 221 | -0.762 | -19.439 | 18.032 | 1.00 | 52.22 | BLGL |
| ATOM | 1639 | C | ARG | 221 | -5.263 | -14.440 | 22.276 | 1.00 | 29.71 | BLGL |
| ATOM | 1640 | O | ARG | 221 | -6.441 | -14.790 | 22.204 | 1.00 | 30.75 | BLGL |
| ATOM | 1641 | N | HIS | 222 | -4.757 | -13.803 | 23.331 | 1.00 | 27.89 | BLGL |
| ATOM | 1642 | CA | HIS | 222 | -5.599 | -13.482 | 24.477 | 1.00 | 27.09 | BLGL |
| ATOM | 1643 | CB | HIS | 222 | -4.844 | -13.728 | 25.782 | 1.00 | 26.93 | BLGL |
| ATOM | 1644 | CG | HIS | 222 | -4.530 | -15.168 | 26.023 | 1.00 | 28.56 | BLGL |
| ATOM | 1645 | CD2 | HIS | 222 | -5.196 | -16.121 | 26.716 | 1.00 | 30.01 | BLGL |
| ATOM | 1646 | ND1 | HIS | 222 | -3.441 | -15.797 | 25.459 | 1.00 | 31.08 | BLGL |
| ATOM | 1647 | CE1 | HIS | 222 | -3.448 | -17.076 | 25.792 | 1.00 | 30.75 | BLGL |
| ATOM | 1648 | NE2 | HIS | 222 | -4.504 | -17.298 | 26.554 | 1.00 | 33.11 | BLGL |
| ATOM | 1649 | C | HIS | 222 | -6.159 | -12.064 | 24.456 | 1.00 | 26.57 | BLGL |

# Fig. 4 cont.

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ATOM   1650  O    HIS   222      -6.646  -11.564   25.469  1.00  25.69      BLGL
ATOM   1651  N    HIS   223      -6.084  -11.418   23.300  1.00  25.18      BLGL
ATOM   1652  CA   HIS   223      -6.627  -10.082   23.151  1.00  26.33      BLGL
ATOM   1653  CB   HIS   223      -8.147  -10.149   23.214  1.00  30.76      BLGL
ATOM   1654  CG   HIS   223      -8.739  -11.182   22.309  1.00  38.88      BLGL
ATOM   1655  CD2  HIS   223      -9.524  -12.253   22.570  1.00  41.07      BLGL
ATOM   1656  ND1  HIS   223      -8.531  -11.182   20.945  1.00  43.14      BLGL
ATOM   1657  CE1  HIS   223      -9.161  -12.210   20.405  1.00  43.27      BLGL
ATOM   1658  NE2  HIS   223      -9.771  -12.876   21.370  1.00  45.48      BLGL
ATOM   1659  C    HIS   223      -6.149   -9.081   24.186  1.00  26.02      BLGL
ATOM   1660  O    HIS   223      -6.961   -8.345   24.750  1.00  27.73      BLGL
ATOM   1661  N    VAL   224      -4.846   -9.044   24.446  1.00  22.81      BLGL
ATOM   1662  CA   VAL   224      -4.316   -8.096   25.413  1.00  18.14      BLGL
ATOM   1663  CB   VAL   224      -2.912   -8.499   25.895  1.00  16.94      BLGL
ATOM   1664  CG1  VAL   224      -2.312   -7.399   26.758  1.00  12.94      BLGL
ATOM   1665  CG2  VAL   224      -2.998   -9.783   26.676  1.00  15.42      BLGL
ATOM   1666  C    VAL   224      -4.241   -6.742   24.734  1.00  17.57      BLGL
ATOM   1667  O    VAL   224      -3.683   -6.610   23.646  1.00  16.83      BLGL
ATOM   1668  N    ASP   225      -4.808   -5.738   25.386  1.00  16.35      BLGL
ATOM   1669  CA   ASP   225      -4.820   -4.393   24.849  1.00  17.47      BLGL
ATOM   1670  CB   ASP   225      -6.123   -3.707   25.254  1.00  17.33      BLGL
ATOM   1671  CG   ASP   225      -6.172   -2.260   24.843  1.00  19.19      BLGL
ATOM   1672  OD1  ASP   225      -5.722   -1.945   23.717  1.00  21.14      BLGL
ATOM   1673  OD2  ASP   225      -6.672   -1.444   25.643  1.00  19.74      BLGL
ATOM   1674  C    ASP   225      -3.626   -3.562   25.306  1.00  18.47      BLGL
ATOM   1675  O    ASP   225      -3.609   -3.073   26.433  1.00  19.94      BLGL
ATOM   1676  N    TYR   226      -2.626   -3.415   24.440  1.00  17.31      BLGL
ATOM   1677  CA   TYR   226      -1.441   -2.610   24.762  1.00  19.05      BLGL
ATOM   1678  CB   TYR   226      -0.315   -3.483   25.359  1.00  17.31      BLGL
ATOM   1679  CG   TYR   226       0.380   -4.417   24.386  1.00  17.91      BLGL
ATOM   1680  CD1  TYR   226      -0.315   -5.469   23.780  1.00  17.20      BLGL
ATOM   1681  CE1  TYR   226       0.317   -6.338   22.891  1.00  14.85      BLGL
ATOM   1682  CD2  TYR   226       1.737   -4.253   24.076  1.00  15.96      BLGL
ATOM   1683  CE2  TYR   226       2.380   -5.117   23.184  1.00  15.01      BLGL
ATOM   1684  CZ   TYR   226       1.661   -6.156   22.598  1.00  16.47      BLGL
ATOM   1685  OH   TYR   226       2.279   -7.019   21.725  1.00  13.64      BLGL
ATOM   1686  C    TYR   226      -0.944   -1.877   23.513  1.00  17.95      BLGL
ATOM   1687  O    TYR   226      -1.285   -2.251   22.398  1.00  17.24      BLGL
ATOM   1688  N    ASP   227      -0.141   -0.836   23.697  1.00  18.09      BLGL
ATOM   1689  CA   ASP   227       0.361   -0.075   22.557  1.00  20.63      BLGL
ATOM   1690  CB   ASP   227       0.126    1.424   22.760  1.00  23.61      BLGL
ATOM   1691  CG   ASP   227      -1.247    1.736   23.282  1.00  24.31      BLGL
ATOM   1692  OD1  ASP   227      -2.242    1.427   22.597  1.00  26.42      BLGL
ATOM   1693  OD2  ASP   227      -1.327    2.298   24.388  1.00  29.59      BLGL
ATOM   1694  C    ASP   227       1.846   -0.263   22.289  1.00  21.20      BLGL
ATOM   1695  O    ASP   227       2.283   -0.241   21.141  1.00  21.63      BLGL
ATOM   1696  N    VAL   228       2.626   -0.432   23.350  1.00  21.33      BLGL
ATOM   1697  CA   VAL   228       4.069   -0.571   23.205  1.00  18.22      BLGL
ATOM   1698  CB   VAL   228       4.822    0.572   23.961  1.00  16.56      BLGL
ATOM   1699  CG1  VAL   228       6.307    0.511   23.669  1.00  16.51      BLGL
ATOM   1700  CG2  VAL   228       4.268    1.921   23.569  1.00  16.96      BLGL
ATOM   1701  C    VAL   228       4.631   -1.892   23.700  1.00  16.80      BLGL
ATOM   1702  O    VAL   228       4.338   -2.338   24.811  1.00  16.77      BLGL
ATOM   1703  N    PHE   229       5.444   -2.510   22.858  1.00  15.66      BLGL
ATOM   1704  CA   PHE   229       6.115   -3.747   23.213  1.00  16.03      BLGL
ATOM   1705  CB   PHE   229       6.177   -4.694   22.007  1.00  15.71      BLGL
ATOM   1706  CG   PHE   229       6.773   -6.038   22.323  1.00  18.72      BLGL
ATOM   1707  CD1  PHE   229       8.148   -6.193   22.458  1.00  20.15      BLGL
ATOM   1708  CD2  PHE   229       5.957   -7.141   22.537  1.00  19.69      BLGL
ATOM   1709  CE1  PHE   229       8.698   -7.424   22.805  1.00  20.33      BLGL
ATOM   1710  CE2  PHE   229       6.502   -8.376   22.885  1.00  19.99      BLGL
ATOM   1711  CZ   PHE   229       7.873   -8.516   23.020  1.00  20.18      BLGL
ATOM   1712  C    PHE   229       7.517   -3.278   23.608  1.00  15.51      BLGL
ATOM   1713  O    PHE   229       8.336   -2.965   22.747  1.00  16.80      BLGL
ATOM   1714  N    ALA   230       7.781   -3.205   24.909  1.00  14.48      BLGL
ATOM   1715  CA   ALA   230       9.076   -2.740   25.392  1.00  16.32      BLGL
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# Fig. 4 cont.

| ATOM | 1716 | CB  | ALA | 230 | 8.892  | -1.878  | 26.632 | 1.00 | 15.48 | BLGL |
|------|------|-----|-----|-----|--------|---------|--------|------|-------|------|
| ATOM | 1717 | C   | ALA | 230 | 10.040 | -3.878  | 25.691 | 1.00 | 17.75 | BLGL |
| ATOM | 1718 | O   | ALA | 230 | 9.624  | -4.990  | 26.019 | 1.00 | 19.06 | BLGL |
| ATOM | 1719 | N   | SER | 231 | 11.334 | -3.588  | 25.580 | 1.00 | 15.44 | BLGL |
| ATOM | 1720 | CA  | SER | 231 | 12.363 | -4.583  | 25.829 | 1.00 | 15.19 | BLGL |
| ATOM | 1721 | CB  | SER | 231 | 12.863 | -5.165  | 24.498 | 1.00 | 12.54 | BLGL |
| ATOM | 1722 | OG  | SER | 231 | 13.966 | -6.035  | 24.696 | 1.00 | 9.34  | BLGL |
| ATOM | 1723 | C   | SER | 231 | 13.554 | -4.024  | 26.601 | 1.00 | 16.12 | BLGL |
| ATOM | 1724 | O   | SER | 231 | 13.915 | -2.852  | 26.463 | 1.00 | 17.19 | BLGL |
| ATOM | 1725 | N   | SER | 232 | 14.152 | -4.865  | 27.434 | 1.00 | 14.04 | BLGL |
| ATOM | 1726 | CA  | SER | 232 | 15.341 | -4.463  | 28.159 | 1.00 | 15.04 | BLGL |
| ATOM | 1727 | CB  | SER | 232 | 15.505 | -5.272  | 29.447 | 1.00 | 14.50 | BLGL |
| ATOM | 1728 | OG  | SER | 232 | 14.733 | -4.727  | 30.499 | 1.00 | 17.36 | BLGL |
| ATOM | 1729 | C   | SER | 232 | 16.485 | -4.810  | 27.216 | 1.00 | 15.02 | BLGL |
| ATOM | 1730 | O   | SER | 232 | 16.354 | -5.696  | 26.374 | 1.00 | 14.13 | BLGL |
| ATOM | 1731 | N   | TYR | 233 | 17.591 | -4.094  | 27.326 | 1.00 | 14.36 | BLGL |
| ATOM | 1732 | CA  | TYR | 233 | 18.738 | -4.410  | 26.506 | 1.00 | 16.28 | BLGL |
| ATOM | 1733 | CB  | TYR | 233 | 18.721 | -3.697  | 25.152 | 1.00 | 15.72 | BLGL |
| ATOM | 1734 | CG  | TYR | 233 | 19.901 | -4.146  | 24.318 | 1.00 | 18.38 | BLGL |
| ATOM | 1735 | CD1 | TYR | 233 | 19.935 | -5.428  | 23.762 | 1.00 | 17.95 | BLGL |
| ATOM | 1736 | CE1 | TYR | 233 | 21.072 | -5.905  | 23.102 | 1.00 | 17.74 | BLGL |
| ATOM | 1737 | CD2 | TYR | 233 | 21.038 | -3.342  | 24.185 | 1.00 | 19.16 | BLGL |
| ATOM | 1738 | CE2 | TYR | 233 | 22.181 | -3.809  | 23.528 | 1.00 | 18.72 | BLGL |
| ATOM | 1739 | CZ  | TYR | 233 | 22.188 | -5.090  | 22.991 | 1.00 | 20.19 | BLGL |
| ATOM | 1740 | OH  | TYR | 233 | 23.305 | -5.552  | 22.339 | 1.00 | 21.28 | BLGL |
| ATOM | 1741 | C   | TYR | 233 | 20.051 | -4.096  | 27.204 | 1.00 | 18.26 | BLGL |
| ATOM | 1742 | O   | TYR | 233 | 20.488 | -2.941  | 27.282 | 1.00 | 19.11 | BLGL |
| ATOM | 1743 | N   | TYR | 234 | 20.672 | -5.148  | 27.715 | 1.00 | 18.61 | BLGL |
| ATOM | 1744 | CA  | TYR | 234 | 21.951 | -5.047  | 28.382 | 1.00 | 20.22 | BLGL |
| ATOM | 1745 | CB  | TYR | 234 | 21.838 | -5.594  | 29.794 | 1.00 | 18.03 | BLGL |
| ATOM | 1746 | CG  | TYR | 234 | 21.020 | -4.689  | 30.678 | 1.00 | 19.42 | BLGL |
| ATOM | 1747 | CD1 | TYR | 234 | 21.536 | -3.473  | 31.130 | 1.00 | 17.03 | BLGL |
| ATOM | 1748 | CE1 | TYR | 234 | 20.778 | -2.628  | 31.935 | 1.00 | 15.84 | BLGL |
| ATOM | 1749 | CD2 | TYR | 234 | 19.718 | -5.035  | 31.051 | 1.00 | 20.59 | BLGL |
| ATOM | 1750 | CE2 | TYR | 234 | 18.950 | -4.194  | 31.854 | 1.00 | 18.88 | BLGL |
| ATOM | 1751 | CZ  | TYR | 234 | 19.489 | -2.995  | 32.294 | 1.00 | 17.70 | BLGL |
| ATOM | 1752 | OH  | TYR | 234 | 18.745 | -2.180  | 33.108 | 1.00 | 17.67 | BLGL |
| ATOM | 1753 | C   | TYR | 234 | 22.896 | -5.875  | 27.538 | 1.00 | 20.87 | BLGL |
| ATOM | 1754 | O   | TYR | 234 | 22.858 | -7.104  | 27.570 | 1.00 | 23.14 | BLGL |
| ATOM | 1755 | N   | PRO | 235 | 23.749 | -5.201  | 26.756 | 1.00 | 21.55 | BLGL |
| ATOM | 1756 | CD  | PRO | 235 | 23.983 | -3.751  | 26.857 | 1.00 | 21.91 | BLGL |
| ATOM | 1757 | CA  | PRO | 235 | 24.728 | -5.825  | 25.864 | 1.00 | 22.81 | BLGL |
| ATOM | 1758 | CB  | PRO | 235 | 25.551 | -4.639  | 25.367 | 1.00 | 22.48 | BLGL |
| ATOM | 1759 | CG  | PRO | 235 | 25.422 | -3.640  | 26.471 | 1.00 | 21.97 | BLGL |
| ATOM | 1760 | C   | PRO | 235 | 25.575 | -6.912  | 26.508 | 1.00 | 23.83 | BLGL |
| ATOM | 1761 | O   | PRO | 235 | 26.118 | -7.762  | 25.812 | 1.00 | 26.44 | BLGL |
| ATOM | 1762 | N   | PHE | 236 | 25.673 | -6.894  | 27.834 | 1.00 | 24.38 | BLGL |
| ATOM | 1763 | CA  | PHE | 236 | 26.451 | -7.894  | 28.556 | 1.00 | 23.56 | BLGL |
| ATOM | 1764 | CB  | PHE | 236 | 26.439 | -7.613  | 30.069 | 1.00 | 22.41 | BLGL |
| ATOM | 1765 | CG  | PHE | 236 | 26.751 | -6.190  | 30.432 | 1.00 | 20.97 | BLGL |
| ATOM | 1766 | CD1 | PHE | 236 | 25.769 | -5.363  | 30.960 | 1.00 | 22.30 | BLGL |
| ATOM | 1767 | CD2 | PHE | 236 | 28.018 | -5.666  | 30.224 | 1.00 | 21.90 | BLGL |
| ATOM | 1768 | CE1 | PHE | 236 | 26.043 | -4.031  | 31.274 | 1.00 | 20.76 | BLGL |
| ATOM | 1769 | CE2 | PHE | 236 | 28.304 | -4.335  | 30.534 | 1.00 | 22.34 | BLGL |
| ATOM | 1770 | CZ  | PHE | 236 | 27.310 | -3.518  | 31.060 | 1.00 | 22.41 | BLGL |
| ATOM | 1771 | C   | PHE | 236 | 25.901 | -9.297  | 28.322 | 1.00 | 24.55 | BLGL |
| ATOM | 1772 | O   | PHE | 236 | 26.664 | -10.252 | 28.209 | 1.00 | 26.43 | BLGL |
| ATOM | 1773 | N   | TRP | 237 | 24.581 | -9.425  | 28.226 | 1.00 | 25.33 | BLGL |
| ATOM | 1774 | CA  | TRP | 237 | 23.971 | -10.745 | 28.067 | 1.00 | 26.98 | BLGL |
| ATOM | 1775 | CB  | TRP | 237 | 23.270 | -11.144 | 29.367 | 1.00 | 27.82 | BLGL |
| ATOM | 1776 | CG  | TRP | 237 | 23.960 | -10.698 | 30.606 | 1.00 | 30.90 | BLGL |
| ATOM | 1777 | CD2 | TRP | 237 | 23.562 | -9.632  | 31.466 | 1.00 | 31.06 | BLGL |
| ATOM | 1778 | CE2 | TRP | 237 | 24.489 | -9.585  | 32.535 | 1.00 | 31.99 | BLGL |
| ATOM | 1779 | CE3 | TRP | 237 | 22.511 | -8.711  | 31.443 | 1.00 | 32.34 | BLGL |
| ATOM | 1780 | CD1 | TRP | 237 | 25.084 | -11.238 | 31.162 | 1.00 | 33.44 | BLGL |
| ATOM | 1781 | NE1 | TRP | 237 | 25.408 | -10.577 | 32.324 | 1.00 | 32.26 | BLGL |

# Fig. 4 cont.

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| ATOM | 1782 | CZ2 | TRP | 237 | 24.396 | -8.652 | 33.570 | 1.00 | 32.74 | BLGL |
|------|------|-----|-----|-----|--------|--------|--------|------|-------|------|
| ATOM | 1783 | CZ3 | TRP | 237 | 22.417 | -7.780 | 32.477 | 1.00 | 34.34 | BLGL |
| ATOM | 1784 | CH2 | TRP | 237 | 23.357 | -7.761 | 33.526 | 1.00 | 33.93 | BLGL |
| ATOM | 1785 | C | TRP | 237 | 22.938 | -10.894 | 26.960 | 1.00 | 26.05 | BLGL |
| ATOM | 1786 | O | TRP | 237 | 22.632 | -12.011 | 26.543 | 1.00 | 25.25 | BLGL |
| ATOM | 1787 | N | HIS | 238 | 22.401 | -9.778 | 26.487 | 1.00 | 24.70 | BLGL |
| ATOM | 1788 | CA | HIS | 238 | 21.333 | -9.824 | 25.504 | 1.00 | 20.96 | BLGL |
| ATOM | 1789 | CB | HIS | 238 | 20.358 | -8.703 | 25.824 | 1.00 | 19.05 | BLGL |
| ATOM | 1790 | CG | HIS | 238 | 19.772 | -8.821 | 27.192 | 1.00 | 17.38 | BLGL |
| ATOM | 1791 | CD2 | HIS | 238 | 19.601 | -9.900 | 27.990 | 1.00 | 16.73 | BLGL |
| ATOM | 1792 | ND1 | HIS | 238 | 19.291 | -7.743 | 27.896 | 1.00 | 20.29 | BLGL |
| ATOM | 1793 | CE1 | HIS | 238 | 18.850 | -8.151 | 29.073 | 1.00 | 20.03 | BLGL |
| ATOM | 1794 | NE2 | HIS | 238 | 19.026 | -9.456 | 29.154 | 1.00 | 19.52 | BLGL |
| ATOM | 1795 | C | HIS | 238 | 21.628 | -9.863 | 24.019 | 1.00 | 20.65 | BLGL |
| ATOM | 1796 | O | HIS | 238 | 20.854 | -9.354 | 23.217 | 1.00 | 22.38 | BLGL |
| ATOM | 1797 | N | GLY | 239 | 22.730 | -10.489 | 23.643 | 1.00 | 19.61 | BLGL |
| ATOM | 1798 | CA | GLY | 239 | 23.037 | -10.607 | 22.234 | 1.00 | 19.09 | BLGL |
| ATOM | 1799 | C | GLY | 239 | 23.345 | -9.338 | 21.474 | 1.00 | 18.09 | BLGL |
| ATOM | 1800 | O | GLY | 239 | 23.535 | -8.271 | 22.046 | 1.00 | 17.84 | BLGL |
| ATOM | 1801 | N | THR | 240 | 23.369 | -9.476 | 20.158 | 1.00 | 17.37 | BLGL |
| ATOM | 1802 | CA | THR | 240 | 23.697 | -8.387 | 19.258 | 1.00 | 18.95 | BLGL |
| ATOM | 1803 | CB | THR | 240 | 24.139 | -8.949 | 17.896 | 1.00 | 18.49 | BLGL |
| ATOM | 1804 | OG1 | THR | 240 | 23.028 | -9.589 | 17.262 | 1.00 | 18.33 | BLGL |
| ATOM | 1805 | CG2 | THR | 240 | 25.239 | -9.964 | 18.076 | 1.00 | 14.06 | BLGL |
| ATOM | 1806 | C | THR | 240 | 22.610 | -7.348 | 19.003 | 1.00 | 20.98 | BLGL |
| ATOM | 1807 | O | THR | 240 | 21.418 | -7.604 | 19.169 | 1.00 | 19.90 | BLGL |
| ATOM | 1808 | N | LEU | 241 | 23.043 | -6.165 | 18.581 | 1.00 | 21.55 | BLGL |
| ATOM | 1809 | CA | LEU | 241 | 22.115 | -5.094 | 18.277 | 1.00 | 21.65 | BLGL |
| ATOM | 1810 | CB | LEU | 241 | 22.874 | -3.780 | 18.086 | 1.00 | 20.04 | BLGL |
| ATOM | 1811 | CG | LEU | 241 | 23.464 | -3.205 | 19.381 | 1.00 | 21.24 | BLGL |
| ATOM | 1812 | CD1 | LEU | 241 | 24.455 | -2.105 | 19.074 | 1.00 | 18.53 | BLGL |
| ATOM | 1813 | CD2 | LEU | 241 | 22.339 | -2.689 | 20.259 | 1.00 | 19.54 | BLGL |
| ATOM | 1814 | C | LEU | 241 | 21.350 | -5.458 | 17.011 | 1.00 | 22.88 | BLGL |
| ATOM | 1815 | O | LEU | 241 | 20.213 | -5.043 | 16.827 | 1.00 | 23.81 | BLGL |
| ATOM | 1816 | N | LYS | 242 | 21.971 | -6.248 | 16.143 | 1.00 | 23.90 | BLGL |
| ATOM | 1817 | CA | LYS | 242 | 21.322 | -6.659 | 14.902 | 1.00 | 25.71 | BLGL |
| ATOM | 1818 | CB | LYS | 242 | 22.314 | -7.426 | 14.025 | 1.00 | 30.56 | BLGL |
| ATOM | 1819 | CG | LYS | 242 | 21.771 | -7.855 | 12.670 | 1.00 | 36.92 | BLGL |
| ATOM | 1820 | CD | LYS | 242 | 22.735 | -8.821 | 11.983 | 1.00 | 43.60 | BLGL |
| ATOM | 1821 | CE | LYS | 242 | 22.175 | -9.333 | 10.664 | 1.00 | 48.93 | BLGL |
| ATOM | 1822 | NZ | LYS | 242 | 21.895 | -8.217 | 9.709 | 1.00 | 51.96 | BLGL |
| ATOM | 1823 | C | LYS | 242 | 20.108 | -7.537 | 15.208 | 1.00 | 24.37 | BLGL |
| ATOM | 1824 | O | LYS | 242 | 19.070 | -7.444 | 14.551 | 1.00 | 23.45 | BLGL |
| ATOM | 1825 | N | ASN | 243 | 20.248 | -8.384 | 16.219 | 1.00 | 23.09 | BLGL |
| ATOM | 1826 | CA | ASN | 243 | 19.178 | -9.279 | 16.637 | 1.00 | 21.13 | BLGL |
| ATOM | 1827 | CB | ASN | 243 | 19.716 | -10.285 | 17.653 | 1.00 | 20.66 | BLGL |
| ATOM | 1828 | CG | ASN | 243 | 18.639 | -11.196 | 18.185 | 1.00 | 22.04 | BLGL |
| ATOM | 1829 | OD1 | ASN | 243 | 18.181 | -12.102 | 17.495 | 1.00 | 21.37 | BLGL |
| ATOM | 1830 | ND2 | ASN | 243 | 18.215 | -10.951 | 19.415 | 1.00 | 21.96 | BLGL |
| ATOM | 1831 | C | ASN | 243 | 18.041 | -8.477 | 17.264 | 1.00 | 21.16 | BLGL |
| ATOM | 1832 | O | ASN | 243 | 16.861 | -8.684 | 16.957 | 1.00 | 18.33 | BLGL |
| ATOM | 1833 | N | LEU | 244 | 18.408 | -7.557 | 18.151 | 1.00 | 20.72 | BLGL |
| ATOM | 1834 | CA | LEU | 244 | 17.429 | -6.712 | 18.821 | 1.00 | 19.78 | BLGL |
| ATOM | 1835 | CB | LEU | 244 | 18.131 | -5.667 | 19.695 | 1.00 | 18.01 | BLGL |
| ATOM | 1836 | CG | LEU | 244 | 17.188 | -4.669 | 20.372 | 1.00 | 16.83 | BLGL |
| ATOM | 1837 | CD1 | LEU | 244 | 16.393 | -5.385 | 21.463 | 1.00 | 13.98 | BLGL |
| ATOM | 1838 | CD2 | LEU | 244 | 17.995 | -3.515 | 20.950 | 1.00 | 16.04 | BLGL |
| ATOM | 1839 | C | LEU | 244 | 16.565 | -6.000 | 17.792 | 1.00 | 19.53 | BLGL |
| ATOM | 1840 | O | LEU | 244 | 15.341 | -6.054 | 17.853 | 1.00 | 20.39 | BLGL |
| ATOM | 1841 | N | THR | 245 | 17.214 | -5.332 | 16.846 | 1.00 | 18.73 | BLGL |
| ATOM | 1842 | CA | THR | 245 | 16.505 | -4.606 | 15.810 | 1.00 | 18.66 | BLGL |
| ATOM | 1843 | CB | THR | 245 | 17.474 | -3.996 | 14.785 | 1.00 | 19.64 | BLGL |
| ATOM | 1844 | OG1 | THR | 245 | 18.318 | -3.037 | 15.430 | 1.00 | 21.51 | BLGL |
| ATOM | 1845 | CG2 | THR | 245 | 16.697 | -3.311 | 13.664 | 1.00 | 17.47 | BLGL |
| ATOM | 1846 | C | THR | 245 | 15.574 | -5.531 | 15.062 | 1.00 | 19.92 | BLGL |
| ATOM | 1847 | O | THR | 245 | 14.410 | -5.219 | 14.834 | 1.00 | 21.53 | BLGL |

# Fig. 4 cont.

| ATOM | 1848 | N | SER | 246 | 16.109 | -6.678 | 14.678 | 1.00 | 20.39 | BLGL |
|------|------|------|-----|-----|--------|--------|--------|------|-------|------|
| ATOM | 1849 | CA | SER | 246 | 15.361 | -7.661 | 13.927 | 1.00 | 19.04 | BLGL |
| ATOM | 1850 | CB | SER | 246 | 16.303 | -8.792 | 13.538 | 1.00 | 18.29 | BLGL |
| ATOM | 1851 | OG | SER | 246 | 15.593 | -9.911 | 13.053 | 1.00 | 23.84 | BLGL |
| ATOM | 1852 | C | SER | 246 | 14.164 | -8.205 | 14.695 | 1.00 | 20.89 | BLGL |
| ATOM | 1853 | O | SER | 246 | 13.034 | -8.169 | 14.214 | 1.00 | 22.76 | BLGL |
| ATOM | 1854 | N | VAL | 247 | 14.411 | -8.703 | 15.899 | 1.00 | 21.65 | BLGL |
| ATOM | 1855 | CA | VAL | 247 | 13.343 | -9.280 | 16.701 | 1.00 | 21.83 | BLGL |
| ATOM | 1856 | CB | VAL | 247 | 13.923 | -9.883 | 18.005 | 1.00 | 20.50 | BLGL |
| ATOM | 1857 | CG1 | VAL | 247 | 14.342 | -8.786 | 18.962 | 1.00 | 20.71 | BLGL |
| ATOM | 1858 | CG2 | VAL | 247 | 12.912 | -10.800 | 18.636 | 1.00 | 23.56 | BLGL |
| ATOM | 1859 | C | VAL | 247 | 12.215 | -8.275 | 17.006 | 1.00 | 22.43 | BLGL |
| ATOM | 1860 | O | VAL | 247 | 11.031 | -8.631 | 17.000 | 1.00 | 22.15 | BLGL |
| ATOM | 1861 | N | LEU | 248 | 12.578 | -7.020 | 17.255 | 1.00 | 22.41 | BLGL |
| ATOM | 1862 | CA | LEU | 248 | 11.584 | -5.990 | 17.538 | 1.00 | 22.55 | BLGL |
| ATOM | 1863 | CB | LEU | 248 | 12.251 | -4.734 | 18.125 | 1.00 | 20.88 | BLGL |
| ATOM | 1864 | CG | LEU | 248 | 12.778 | -4.816 | 19.563 | 1.00 | 19.44 | BLGL |
| ATOM | 1865 | CD1 | LEU | 248 | 13.426 | -3.498 | 19.954 | 1.00 | 17.12 | BLGL |
| ATOM | 1866 | CD2 | LEU | 248 | 11.639 | -5.143 | 20.505 | 1.00 | 15.29 | BLGL |
| ATOM | 1867 | C | LEU | 248 | 10.805 | -5.617 | 16.270 | 1.00 | 23.02 | BLGL |
| ATOM | 1868 | O | LEU | 248 | 9.597 | -5.381 | 16.318 | 1.00 | 22.01 | BLGL |
| ATOM | 1869 | N | THR | 249 | 11.496 | -5.570 | 15.136 | 1.00 | 20.49 | BLGL |
| ATOM | 1870 | CA | THR | 249 | 10.844 | -5.220 | 13.890 | 1.00 | 21.29 | BLGL |
| ATOM | 1871 | CB | THR | 249 | 11.836 | -5.197 | 12.722 | 1.00 | 22.20 | BLGL |
| ATOM | 1872 | OG1 | THR | 249 | 12.872 | -4.246 | 12.994 | 1.00 | 24.83 | BLGL |
| ATOM | 1873 | CG2 | THR | 249 | 11.128 | -4.808 | 11.440 | 1.00 | 20.47 | BLGL |
| ATOM | 1874 | C | THR | 249 | 9.739 | -6.214 | 13.573 | 1.00 | 22.84 | BLGL |
| ATOM | 1875 | O | THR | 249 | 8.706 | -5.842 | 13.020 | 1.00 | 20.69 | BLGL |
| ATOM | 1876 | N | SER | 250 | 9.956 | -7.481 | 13.920 | 1.00 | 23.97 | BLGL |
| ATOM | 1877 | CA | SER | 250 | 8.945 | -8.509 | 13.667 | 1.00 | 25.77 | BLGL |
| ATOM | 1878 | CB | SER | 250 | 9.451 | -9.889 | 14.076 | 1.00 | 27.18 | BLGL |
| ATOM | 1879 | OG | SER | 250 | 10.487 | -10.310 | 13.213 | 1.00 | 34.71 | BLGL |
| ATOM | 1880 | C | SER | 250 | 7.686 | -8.196 | 14.446 | 1.00 | 24.53 | BLGL |
| ATOM | 1881 | O | SER | 250 | 6.590 | -8.207 | 13.892 | 1.00 | 24.89 | BLGL |
| ATOM | 1882 | N | VAL | 251 | 7.850 | -7.919 | 15.736 | 1.00 | 22.02 | BLGL |
| ATOM | 1883 | CA | VAL | 251 | 6.713 | -7.592 | 16.581 | 1.00 | 20.32 | BLGL |
| ATOM | 1884 | CB | VAL | 251 | 7.156 | -7.246 | 18.022 | 1.00 | 19.00 | BLGL |
| ATOM | 1885 | CG1 | VAL | 251 | 5.972 | -6.733 | 18.822 | 1.00 | 19.03 | BLGL |
| ATOM | 1886 | CG2 | VAL | 251 | 7.736 | -8.475 | 18.693 | 1.00 | 17.23 | BLGL |
| ATOM | 1887 | C | VAL | 251 | 5.968 | -6.401 | 15.984 | 1.00 | 20.70 | BLGL |
| ATOM | 1888 | O | VAL | 251 | 4.741 | -6.399 | 15.912 | 1.00 | 20.26 | BLGL |
| ATOM | 1889 | N | ALA | 252 | 6.717 | -5.396 | 15.546 | 1.00 | 20.84 | BLGL |
| ATOM | 1890 | CA | ALA | 252 | 6.123 | -4.198 | 14.965 | 1.00 | 21.97 | BLGL |
| ATOM | 1891 | CB | ALA | 252 | 7.203 | -3.175 | 14.663 | 1.00 | 21.24 | BLGL |
| ATOM | 1892 | C | ALA | 252 | 5.330 | -4.497 | 13.701 | 1.00 | 22.61 | BLGL |
| ATOM | 1893 | O | ALA | 252 | 4.137 | -4.219 | 13.629 | 1.00 | 23.36 | BLGL |
| ATOM | 1894 | N | ASP | 253 | 5.999 | -5.069 | 12.711 | 1.00 | 22.58 | BLGL |
| ATOM | 1895 | CA | ASP | 253 | 5.366 | -5.386 | 11.440 | 1.00 | 23.48 | BLGL |
| ATOM | 1896 | CB | ASP | 253 | 6.394 | -5.968 | 10.472 | 1.00 | 23.27 | BLGL |
| ATOM | 1897 | CG | ASP | 253 | 7.403 | -4.946 | 10.019 | 1.00 | 25.67 | BLGL |
| ATOM | 1898 | OD1 | ASP | 253 | 8.372 | -5.346 | 9.337 | 1.00 | 26.60 | BLGL |
| ATOM | 1899 | OD2 | ASP | 253 | 7.224 | -3.744 | 10.344 | 1.00 | 27.47 | BLGL |
| ATOM | 1900 | C | ASP | 253 | 4.203 | -6.352 | 11.556 | 1.00 | 24.77 | BLGL |
| ATOM | 1901 | O | ASP | 253 | 3.174 | -6.174 | 10.904 | 1.00 | 25.85 | BLGL |
| ATOM | 1902 | N | THR | 254 | 4.359 | -7.371 | 12.389 | 1.00 | 24.09 | BLGL |
| ATOM | 1903 | CA | THR | 254 | 3.317 | -8.374 | 12.537 | 1.00 | 22.38 | BLGL |
| ATOM | 1904 | CB | THR | 254 | 3.892 | -9.679 | 13.094 | 1.00 | 21.12 | BLGL |
| ATOM | 1905 | OG1 | THR | 254 | 5.000 | -10.096 | 12.287 | 1.00 | 22.06 | BLGL |
| ATOM | 1906 | CG2 | THR | 254 | 2.836 | -10.765 | 13.073 | 1.00 | 20.31 | BLGL |
| ATOM | 1907 | C | THR | 254 | 2.123 | -7.977 | 13.395 | 1.00 | 23.11 | BLGL |
| ATOM | 1908 | O | THR | 254 | 0.995 | -8.366 | 13.102 | 1.00 | 26.89 | BLGL |
| ATOM | 1909 | N | TYR | 255 | 2.345 | -7.201 | 14.444 | 1.00 | 21.45 | BLGL |
| ATOM | 1910 | CA | TYR | 255 | 1.231 | -6.835 | 15.307 | 1.00 | 20.15 | BLGL |
| ATOM | 1911 | CB | TYR | 255 | 1.488 | -7.377 | 16.709 | 1.00 | 20.87 | BLGL |
| ATOM | 1912 | CG | TYR | 255 | 1.670 | -8.876 | 16.701 | 1.00 | 22.40 | BLGL |
| ATOM | 1913 | CD1 | TYR | 255 | 0.568 | -9.728 | 16.568 | 1.00 | 21.45 | BLGL |

# Fig. 4 cont.

| ATOM | 1914 | CE1 | TYR | 255 | 0.731 | -11.107 | 16.494 | 1.00 | 21.01 | BLGL |
|------|------|-----|-----|-----|-------|---------|--------|------|-------|------|
| ATOM | 1915 | CD2 | TYR | 255 | 2.943 | -9.443 | 16.761 | 1.00 | 19.96 | BLGL |
| ATOM | 1916 | CE2 | TYR | 255 | 3.117 | -10.822 | 16.686 | 1.00 | 20.59 | BLGL |
| ATOM | 1917 | CZ | TYR | 255 | 2.008 | -11.647 | 16.554 | 1.00 | 21.17 | BLGL |
| ATOM | 1918 | OH | TYR | 255 | 2.179 | -13.009 | 16.495 | 1.00 | 21.44 | BLGL |
| ATOM | 1919 | C | TYR | 255 | 0.927 | -5.357 | 15.360 | 1.00 | 19.29 | BLGL |
| ATOM | 1920 | O | TYR | 255 | 0.056 | -4.923 | 16.104 | 1.00 | 19.71 | BLGL |
| ATOM | 1921 | N | GLY | 256 | 1.649 | -4.585 | 14.562 | 1.00 | 20.06 | BLGL |
| ATOM | 1922 | CA | GLY | 256 | 1.421 | -3.155 | 14.516 | 1.00 | 21.23 | BLGL |
| ATOM | 1923 | C | GLY | 256 | 1.582 | -2.454 | 15.847 | 1.00 | 21.40 | BLGL |
| ATOM | 1924 | O | GLY | 256 | 0.788 | -1.593 | 16.212 | 1.00 | 22.35 | BLGL |
| ATOM | 1925 | N | LYS | 257 | 2.619 | -2.815 | 16.581 | 1.00 | 20.19 | BLGL |
| ATOM | 1926 | CA | LYS | 257 | 2.845 | -2.182 | 17.861 | 1.00 | 21.01 | BLGL |
| ATOM | 1927 | CB | LYS | 257 | 3.032 | -3.244 | 18.949 | 1.00 | 20.86 | BLGL |
| ATOM | 1928 | CG | LYS | 257 | 1.863 | -4.191 | 19.122 | 1.00 | 18.58 | BLGL |
| ATOM | 1929 | CD | LYS | 257 | 0.615 | -3.458 | 19.566 | 1.00 | 17.81 | BLGL |
| ATOM | 1930 | CE | LYS | 257 | -0.524 | -4.428 | 19.765 | 1.00 | 16.84 | BLGL |
| ATOM | 1931 | NZ | LYS | 257 | -1.801 | -3.739 | 20.053 | 1.00 | 19.74 | BLGL |
| ATOM | 1932 | C | LYS | 257 | 4.082 | -1.300 | 17.792 | 1.00 | 20.95 | BLGL |
| ATOM | 1933 | O | LYS | 257 | 4.934 | -1.474 | 16.918 | 1.00 | 19.83 | BLGL |
| ATOM | 1934 | N | LYS | 258 | 4.161 | -0.333 | 18.699 | 1.00 | 19.92 | BLGL |
| ATOM | 1935 | CA | LYS | 258 | 5.329 | 0.526 | 18.771 | 1.00 | 21.02 | BLGL |
| ATOM | 1936 | CB | LYS | 258 | 5.037 | 1.785 | 19.581 | 1.00 | 24.26 | BLGL |
| ATOM | 1937 | CG | LYS | 258 | 3.850 | 2.601 | 19.139 | 1.00 | 27.83 | BLGL |
| ATOM | 1938 | CD | LYS | 258 | 4.143 | 3.387 | 17.887 | 1.00 | 33.22 | BLGL |
| ATOM | 1939 | CE | LYS | 258 | 3.297 | 4.652 | 17.862 | 1.00 | 36.49 | BLGL |
| ATOM | 1940 | NZ | LYS | 258 | 1.845 | 4.362 | 18.036 | 1.00 | 38.07 | BLGL |
| ATOM | 1941 | C | LYS | 258 | 6.322 | -0.326 | 19.559 | 1.00 | 21.33 | BLGL |
| ATOM | 1942 | O | LYS | 258 | 5.923 | -1.248 | 20.276 | 1.00 | 21.62 | BLGL |
| ATOM | 1943 | N | VAL | 259 | 7.607 | -0.037 | 19.430 | 1.00 | 18.75 | BLGL |
| ATOM | 1944 | CA | VAL | 259 | 8.604 | -0.786 | 20.176 | 1.00 | 17.87 | BLGL |
| ATOM | 1945 | CB | VAL | 259 | 9.391 | -1.762 | 19.271 | 1.00 | 17.66 | BLGL |
| ATOM | 1946 | CG1 | VAL | 259 | 8.447 | -2.789 | 18.686 | 1.00 | 16.47 | BLGL |
| ATOM | 1947 | CG2 | VAL | 259 | 10.118 | -0.997 | 18.171 | 1.00 | 16.36 | BLGL |
| ATOM | 1948 | C | VAL | 259 | 9.572 | 0.190 | 20.816 | 1.00 | 18.60 | BLGL |
| ATOM | 1949 | O | VAL | 259 | 9.628 | 1.362 | 20.443 | 1.00 | 19.89 | BLGL |
| ATOM | 1950 | N | MET | 260 | 10.328 | -0.280 | 21.794 | 1.00 | 18.23 | BLGL |
| ATOM | 1951 | CA | MET | 260 | 11.295 | 0.583 | 22.452 | 1.00 | 18.93 | BLGL |
| ATOM | 1952 | CB | MET | 260 | 10.594 | 1.741 | 23.179 | 1.00 | 17.82 | BLGL |
| ATOM | 1953 | CG | MET | 260 | 9.861 | 1.335 | 24.450 | 1.00 | 18.62 | BLGL |
| ATOM | 1954 | SD | MET | 260 | 9.338 | 2.760 | 25.444 | 1.00 | 20.82 | BLGL |
| ATOM | 1955 | CE | MET | 260 | 9.092 | 1.989 | 27.061 | 1.00 | 14.70 | BLGL |
| ATOM | 1956 | C | MET | 260 | 12.109 | -0.200 | 23.461 | 1.00 | 18.97 | BLGL |
| ATOM | 1957 | O | MET | 260 | 11.757 | -1.326 | 23.827 | 1.00 | 18.84 | BLGL |
| ATOM | 1958 | N | VAL | 261 | 13.207 | 0.401 | 23.900 | 1.00 | 18.49 | BLGL |
| ATOM | 1959 | CA | VAL | 261 | 14.049 | -0.215 | 24.907 | 1.00 | 19.01 | BLGL |
| ATOM | 1960 | CB | VAL | 261 | 15.545 | -0.063 | 24.567 | 1.00 | 18.88 | BLGL |
| ATOM | 1961 | CG1 | VAL | 261 | 16.399 | -0.549 | 25.728 | 1.00 | 19.31 | BLGL |
| ATOM | 1962 | CG2 | VAL | 261 | 15.867 | -0.867 | 23.326 | 1.00 | 17.95 | BLGL |
| ATOM | 1963 | C | VAL | 261 | 13.713 | 0.493 | 26.218 | 1.00 | 17.97 | BLGL |
| ATOM | 1964 | O | VAL | 261 | 13.854 | 1.712 | 26.343 | 1.00 | 14.60 | BLGL |
| ATOM | 1965 | N | ALA | 262 | 13.228 | -0.280 | 27.180 | 1.00 | 18.80 | BLGL |
| ATOM | 1966 | CA | ALA | 262 | 12.846 | 0.269 | 28.473 | 1.00 | 21.56 | BLGL |
| ATOM | 1967 | CB | ALA | 262 | 11.777 | -0.617 | 29.107 | 1.00 | 20.01 | BLGL |
| ATOM | 1968 | C | ALA | 262 | 14.047 | 0.409 | 29.412 | 1.00 | 21.77 | BLGL |
| ATOM | 1969 | O | ALA | 262 | 14.079 | 1.297 | 30.262 | 1.00 | 22.42 | BLGL |
| ATOM | 1970 | N | GLU | 263 | 15.036 | -0.464 | 29.247 | 1.00 | 20.47 | BLGL |
| ATOM | 1971 | CA | GLU | 263 | 16.214 | -0.433 | 30.091 | 1.00 | 19.18 | BLGL |
| ATOM | 1972 | CB | GLU | 263 | 16.099 | -1.464 | 31.211 | 1.00 | 18.99 | BLGL |
| ATOM | 1973 | CG | GLU | 263 | 15.178 | -1.102 | 32.358 | 1.00 | 21.05 | BLGL |
| ATOM | 1974 | CD | GLU | 263 | 15.151 | -2.191 | 33.417 | 1.00 | 19.91 | BLGL |
| ATOM | 1975 | OE1 | GLU | 263 | 16.207 | -2.819 | 33.642 | 1.00 | 20.67 | BLGL |
| ATOM | 1976 | OE2 | GLU | 263 | 14.087 | -2.422 | 34.029 | 1.00 | 22.21 | BLGL |
| ATOM | 1977 | C | GLU | 263 | 17.483 | -0.729 | 29.319 | 1.00 | 19.96 | BLGL |
| ATOM | 1978 | O | GLU | 263 | 17.497 | -1.587 | 28.440 | 1.00 | 20.56 | BLGL |
| ATOM | 1979 | N | THR | 264 | 18.547 | -0.013 | 29.661 | 1.00 | 17.62 | BLGL |

# Fig. 4 cont.

| ATOM | 1980 | CA  | THR | 264 | 19.844 | -0.219 | 29.042 | 1.00 | 15.98 | BLGL |
| ATOM | 1981 | CB  | THR | 264 | 19.874 | 0.247  | 27.573 | 1.00 | 16.21 | BLGL |
| ATOM | 1982 | OG1 | THR | 264 | 20.989 | -0.366 | 26.907 | 1.00 | 15.60 | BLGL |
| ATOM | 1983 | CG2 | THR | 264 | 20.036 | 1.771  | 27.494 | 1.00 | 13.52 | BLGL |
| ATOM | 1984 | C   | THR | 264 | 20.872 | 0.578  | 29.820 | 1.00 | 15.21 | BLGL |
| ATOM | 1985 | O   | THR | 264 | 20.532 | 1.477  | 30.579 | 1.00 | 14.74 | BLGL |
| ATOM | 1986 | N   | SER | 265 | 22.136 | 0.240  | 29.621 | 1.00 | 15.34 | BLGL |
| ATOM | 1987 | CA  | SER | 265 | 23.229 | 0.936  | 30.280 | 1.00 | 16.34 | BLGL |
| ATOM | 1988 | CB  | SER | 265 | 23.113 | 0.819  | 31.802 | 1.00 | 16.26 | BLGL |
| ATOM | 1989 | OG  | SER | 265 | 23.293 | -0.517 | 32.249 | 1.00 | 16.64 | BLGL |
| ATOM | 1990 | C   | SER | 265 | 24.531 | 0.312  | 29.826 | 1.00 | 17.34 | BLGL |
| ATOM | 1991 | O   | SER | 265 | 24.543 | -0.607 | 29.005 | 1.00 | 18.70 | BLGL |
| ATOM | 1992 | N   | TYR | 266 | 25.629 | 0.836  | 30.349 | 1.00 | 18.17 | BLGL |
| ATOM | 1993 | CA  | TYR | 266 | 26.939 | 0.307  | 30.039 | 1.00 | 17.93 | BLGL |
| ATOM | 1994 | CB  | TYR | 266 | 27.397 | 0.699  | 28.640 | 1.00 | 15.84 | BLGL |
| ATOM | 1995 | CG  | TYR | 266 | 28.485 | -0.218 | 28.131 | 1.00 | 17.82 | BLGL |
| ATOM | 1996 | CD1 | TYR | 266 | 28.192 | -1.527 | 27.774 | 1.00 | 18.54 | BLGL |
| ATOM | 1997 | CE1 | TYR | 266 | 29.186 | -2.396 | 27.329 | 1.00 | 19.26 | BLGL |
| ATOM | 1998 | CD2 | TYR | 266 | 29.816 | 0.210  | 28.035 | 1.00 | 20.22 | BLGL |
| ATOM | 1999 | CE2 | TYR | 266 | 30.826 | -0.656 | 27.591 | 1.00 | 19.11 | BLGL |
| ATOM | 2000 | CZ  | TYR | 266 | 30.499 | -1.962 | 27.238 | 1.00 | 19.47 | BLGL |
| ATOM | 2001 | OH  | TYR | 266 | 31.472 | -2.836 | 26.784 | 1.00 | 18.36 | BLGL |
| ATOM | 2002 | C   | TYR | 266 | 27.911 | 0.846  | 31.064 | 1.00 | 18.90 | BLGL |
| ATOM | 2003 | O   | TYR | 266 | 27.681 | 1.895  | 31.665 | 1.00 | 18.09 | BLGL |
| ATOM | 2004 | N   | THR | 267 | 28.995 | 0.105  | 31.259 | 1.00 | 20.38 | BLGL |
| ATOM | 2005 | CA  | THR | 267 | 30.037 | 0.462  | 32.210 | 1.00 | 21.04 | BLGL |
| ATOM | 2006 | CB  | THR | 267 | 30.852 | -0.773 | 32.580 | 1.00 | 20.00 | BLGL |
| ATOM | 2007 | OG1 | THR | 267 | 31.305 | -1.402 | 31.373 | 1.00 | 19.78 | BLGL |
| ATOM | 2008 | CG2 | THR | 267 | 30.017 | -1.752 | 33.366 | 1.00 | 19.30 | BLGL |
| ATOM | 2009 | C   | THR | 267 | 31.000 | 1.482  | 31.619 | 1.00 | 21.49 | BLGL |
| ATOM | 2010 | O   | THR | 267 | 31.455 | 1.315  | 30.488 | 1.00 | 24.81 | BLGL |
| ATOM | 2011 | N   | TYR | 268 | 31.320 | 2.525  | 32.384 | 1.00 | 20.55 | BLGL |
| ATOM | 2012 | CA  | TYR | 268 | 32.268 | 3.546  | 31.933 | 1.00 | 20.98 | BLGL |
| ATOM | 2013 | CB  | TYR | 268 | 31.724 | 4.958  | 32.205 | 1.00 | 21.01 | BLGL |
| ATOM | 2014 | CG  | TYR | 268 | 31.844 | 5.439  | 33.639 | 1.00 | 19.32 | BLGL |
| ATOM | 2015 | CD1 | TYR | 268 | 33.019 | 6.027  | 34.105 | 1.00 | 20.87 | BLGL |
| ATOM | 2016 | CE1 | TYR | 268 | 33.129 | 6.471  | 35.426 | 1.00 | 20.17 | BLGL |
| ATOM | 2017 | CD2 | TYR | 268 | 30.778 | 5.302  | 34.532 | 1.00 | 21.37 | BLGL |
| ATOM | 2018 | CE2 | TYR | 268 | 30.873 | 5.739  | 35.853 | 1.00 | 19.23 | BLGL |
| ATOM | 2019 | CZ  | TYR | 268 | 32.049 | 6.322  | 36.295 | 1.00 | 21.74 | BLGL |
| ATOM | 2020 | OH  | TYR | 268 | 32.137 | 6.753  | 37.604 | 1.00 | 22.30 | BLGL |
| ATOM | 2021 | C   | TYR | 268 | 33.597 | 3.364  | 32.664 | 1.00 | 21.83 | BLGL |
| ATOM | 2022 | O   | TYR | 268 | 34.590 | 4.013  | 32.344 | 1.00 | 18.94 | BLGL |
| ATOM | 2023 | N   | THR | 269 | 33.600 | 2.479  | 33.657 | 1.00 | 22.82 | BLGL |
| ATOM | 2024 | CA  | THR | 269 | 34.795 | 2.213  | 34.451 | 1.00 | 23.10 | BLGL |
| ATOM | 2025 | CB  | THR | 269 | 34.970 | 3.271  | 35.573 | 1.00 | 20.44 | BLGL |
| ATOM | 2026 | OG1 | THR | 269 | 36.161 | 2.989  | 36.311 | 1.00 | 20.91 | BLGL |
| ATOM | 2027 | CG2 | THR | 269 | 33.791 | 3.250  | 36.524 | 1.00 | 18.84 | BLGL |
| ATOM | 2028 | C   | THR | 269 | 34.693 | 0.834  | 35.083 | 1.00 | 23.00 | BLGL |
| ATOM | 2029 | O   | THR | 269 | 33.607 | 0.376  | 35.403 | 1.00 | 25.15 | BLGL |
| ATOM | 2030 | N   | ALA | 270 | 35.826 | 0.170  | 35.259 | 1.00 | 24.31 | BLGL |
| ATOM | 2031 | CA  | ALA | 270 | 35.825 | -1.158 | 35.853 | 1.00 | 24.71 | BLGL |
| ATOM | 2032 | CB  | ALA | 270 | 37.058 | -1.933 | 35.409 | 1.00 | 21.17 | BLGL |
| ATOM | 2033 | C   | ALA | 270 | 35.810 | -1.019 | 37.361 | 1.00 | 25.78 | BLGL |
| ATOM | 2034 | O   | ALA | 270 | 35.538 | -1.970 | 38.080 | 1.00 | 29.18 | BLGL |
| ATOM | 2035 | N   | GLU | 271 | 36.083 | 0.185  | 37.836 | 1.00 | 27.12 | BLGL |
| ATOM | 2036 | CA  | GLU | 271 | 36.133 | 0.448  | 39.263 | 1.00 | 29.78 | BLGL |
| ATOM | 2037 | CB  | GLU | 271 | 36.914 | 1.742  | 39.495 | 1.00 | 32.08 | BLGL |
| ATOM | 2038 | CG  | GLU | 271 | 36.864 | 2.261  | 40.920 | 1.00 | 35.54 | BLGL |
| ATOM | 2039 | CD  | GLU | 271 | 37.750 | 3.466  | 41.110 | 1.00 | 36.58 | BLGL |
| ATOM | 2040 | OE1 | GLU | 271 | 38.022 | 4.167  | 40.108 | 1.00 | 36.10 | BLGL |
| ATOM | 2041 | OE2 | GLU | 271 | 38.160 | 3.714  | 42.262 | 1.00 | 38.61 | BLGL |
| ATOM | 2042 | C   | GLU | 271 | 34.783 | 0.527  | 39.977 | 1.00 | 30.16 | BLGL |
| ATOM | 2043 | O   | GLU | 271 | 33.776 | 0.938  | 39.405 | 1.00 | 31.60 | BLGL |
| ATOM | 2044 | N   | ASP | 272 | 34.782 | 0.125  | 41.242 | 1.00 | 30.13 | BLGL |
| ATOM | 2045 | CA  | ASP | 272 | 33.590 | 0.169  | 42.081 | 1.00 | 30.63 | BLGL |

# Fig. 4 cont.

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ATOM  2046  CB   ASP  272    33.333  -1.190  42.722  1.00  29.68    BLGL
ATOM  2047  CG   ASP  272    32.488  -1.081  43.968  1.00  29.93    BLGL
ATOM  2048  OD1  ASP  272    31.427  -0.428  43.896  1.00  29.02    BLGL
ATOM  2049  OD2  ASP  272    32.884  -1.640  45.014  1.00  30.80    BLGL
ATOM  2050  C    ASP  272    33.865   1.188  43.178  1.00  31.65    BLGL
ATOM  2051  O    ASP  272    34.705   0.946  44.045  1.00  33.92    BLGL
ATOM  2052  N    GLY  273    33.163   2.318  43.157  1.00  31.58    BLGL
ATOM  2053  CA   GLY  273    33.420   3.340  44.158  1.00  32.18    BLGL
ATOM  2054  C    GLY  273    32.476   3.304  45.333  1.00  31.14    BLGL
ATOM  2055  O    GLY  273    32.407   4.250  46.116  1.00  32.09    BLGL
ATOM  2056  N    ASP  274    31.786   2.184  45.472  1.00  30.99    BLGL
ATOM  2057  CA   ASP  274    30.790   2.002  46.511  1.00  30.40    BLGL
ATOM  2058  CB   ASP  274    29.550   1.377  45.871  1.00  31.29    BLGL
ATOM  2059  CG   ASP  274    28.304   1.620  46.659  1.00  32.35    BLGL
ATOM  2060  OD1  ASP  274    27.319   0.902  46.433  1.00  34.84    BLGL
ATOM  2061  OD2  ASP  274    28.299   2.539  47.495  1.00  38.43    BLGL
ATOM  2062  C    ASP  274    31.264   1.104  47.649  1.00  30.15    BLGL
ATOM  2063  O    ASP  274    31.075   1.408  48.827  1.00  28.39    BLGL
ATOM  2064  N    GLY  275    31.867  -0.017  47.283  1.00  28.33    BLGL
ATOM  2065  CA   GLY  275    32.311  -0.956  48.283  1.00  29.05    BLGL
ATOM  2066  C    GLY  275    31.486  -2.210  48.099  1.00  28.72    BLGL
ATOM  2067  O    GLY  275    31.881  -3.298  48.519  1.00  31.31    BLGL
ATOM  2068  N    HIS  276    30.325  -2.046  47.472  1.00  26.86    BLGL
ATOM  2069  CA   HIS  276    29.431  -3.164  47.191  1.00  24.43    BLGL
ATOM  2070  CB   HIS  276    27.974  -2.726  47.336  1.00  23.89    BLGL
ATOM  2071  CG   HIS  276    26.986  -3.842  47.172  1.00  26.16    BLGL
ATOM  2072  CD2  HIS  276    26.329  -4.297  46.078  1.00  24.85    BLGL
ATOM  2073  ND1  HIS  276    26.595  -4.652  48.217  1.00  26.36    BLGL
ATOM  2074  CE1  HIS  276    25.741  -5.557  47.776  1.00  24.78    BLGL
ATOM  2075  NE2  HIS  276    25.562  -5.363  46.481  1.00  25.01    BLGL
ATOM  2076  C    HIS  276    29.691  -3.597  45.748  1.00  24.24    BLGL
ATOM  2077  O    HIS  276    29.512  -2.808  44.822  1.00  23.66    BLGL
ATOM  2078  N    GLY  277    30.108  -4.844  45.562  1.00  23.41    BLGL
ATOM  2079  CA   GLY  277    30.397  -5.343  44.225  1.00  23.85    BLGL
ATOM  2080  C    GLY  277    29.405  -4.987  43.130  1.00  24.88    BLGL
ATOM  2081  O    GLY  277    28.185  -5.064  43.320  1.00  25.03    BLGL
ATOM  2082  N    ASN  278    29.935  -4.616  41.966  1.00  24.25    BLGL
ATOM  2083  CA   ASN  278    29.114  -4.238  40.822  1.00  22.79    BLGL
ATOM  2084  CB   ASN  278    29.827  -3.150  40.027  1.00  21.96    BLGL
ATOM  2085  CG   ASN  278    29.928  -1.844  40.797  1.00  23.90    BLGL
ATOM  2086  ND2  ASN  278    30.661  -0.934  40.410  1.00  26.25    BLGL
ATOM  2087  OD1  ASN  278    29.177  -1.742  41.889  1.00  21.34    BLGL
ATOM  2088  C    ASN  278    28.748  -5.407  39.910  1.00  23.33    BLGL
ATOM  2089  O    ASN  278    29.408  -6.443  39.898  1.00  22.97    BLGL
ATOM  2090  N    THR  279    27.675  -5.226  39.152  1.00  23.75    BLGL
ATOM  2091  CA   THR  279    27.188  -6.247  38.241  1.00  24.46    BLGL
ATOM  2092  CB   THR  279    25.821  -5.857  37.666  1.00  25.31    BLGL
ATOM  2093  OG1  THR  279    24.874  -5.729  38.728  1.00  27.04    BLGL
ATOM  2094  CG2  THR  279    25.331  -6.910  36.701  1.00  28.22    BLGL
ATOM  2095  C    THR  279    28.137  -6.482  37.078  1.00  24.01    BLGL
ATOM  2096  O    THR  279    28.356  -7.613  36.659  1.00  24.35    BLGL
ATOM  2097  N    ALA  280    28.687  -5.401  36.547  1.00  24.16    BLGL
ATOM  2098  CA   ALA  280    29.599  -5.495  35.422  1.00  24.11    BLGL
ATOM  2099  CB   ALA  280    28.857  -5.182  34.137  1.00  21.63    BLGL
ATOM  2100  C    ALA  280    30.749  -4.512  35.616  1.00  25.17    BLGL
ATOM  2101  O    ALA  280    30.638  -3.565  36.379  1.00  26.21    BLGL
ATOM  2102  N    PRO  281    31.881  -4.766  34.942  1.00  25.93    BLGL
ATOM  2103  CD   PRO  281    32.977  -3.790  34.829  1.00  26.64    BLGL
ATOM  2104  CA   PRO  281    32.106  -5.896  34.037  1.00  27.75    BLGL
ATOM  2105  CB   PRO  281    33.155  -5.353  33.084  1.00  27.25    BLGL
ATOM  2106  CG   PRO  281    34.001  -4.545  33.998  1.00  28.42    BLGL
ATOM  2107  C    PRO  281    32.590  -7.142  34.773  1.00  29.21    BLGL
ATOM  2108  O    PRO  281    33.055  -7.071  35.902  1.00  31.08    BLGL
ATOM  2109  N    LYS  282    32.468  -8.287  34.123  1.00  31.67    BLGL
ATOM  2110  CA   LYS  282    32.902  -9.546  34.705  1.00  35.33    BLGL
ATOM  2111  CB   LYS  282    31.788 -10.169  35.537  1.00  34.90    BLGL
```

# Fig. 4 cont.

| ATOM | 2112 | CG | LYS | 282 | 31.527 | -9.495 | 36.861 | 1.00 | 37.13 | BLGL |
|------|------|-----|-----|-----|--------|--------|--------|------|-------|------|
| ATOM | 2113 | CD | LYS | 282 | 30.496 | -10.301 | 37.636 | 1.00 | 38.88 | BLGL |
| ATOM | 2114 | CE | LYS | 282 | 30.386 | -9.846 | 39.077 | 1.00 | 40.27 | BLGL |
| ATOM | 2115 | NZ | LYS | 282 | 29.540 | -10.796 | 39.851 | 1.00 | 42.22 | BLGL |
| ATOM | 2116 | C | LYS | 282 | 33.270 | -10.495 | 33.583 | 1.00 | 38.11 | BLGL |
| ATOM | 2117 | O | LYS | 282 | 32.931 | -10.251 | 32.429 | 1.00 | 39.52 | BLGL |
| ATOM | 2118 | N | ASN | 283 | 33.967 | -11.575 | 33.920 | 1.00 | 42.82 | BLGL |
| ATOM | 2119 | CA | ASN | 283 | 34.355 | -12.558 | 32.914 | 1.00 | 46.20 | BLGL |
| ATOM | 2120 | CB | ASN | 283 | 35.290 | -13.614 | 33.512 | 1.00 | 50.82 | BLGL |
| ATOM | 2121 | CG | ASN | 283 | 36.534 | -13.010 | 34.122 | 1.00 | 56.85 | BLGL |
| ATOM | 2122 | OD1 | ASN | 283 | 36.474 | -12.369 | 35.175 | 1.00 | 61.22 | BLGL |
| ATOM | 2123 | ND2 | ASN | 283 | 37.672 | -13.200 | 33.461 | 1.00 | 58.97 | BLGL |
| ATOM | 2124 | C | ASN | 283 | 33.100 | -13.246 | 32.382 | 1.00 | 45.60 | BLGL |
| ATOM | 2125 | O | ASN | 283 | 32.163 | -13.532 | 33.138 | 1.00 | 44.14 | BLGL |
| ATOM | 2126 | N | GLY | 284 | 33.081 | -13.507 | 31.080 | 1.00 | 44.05 | BLGL |
| ATOM | 2127 | CA | GLY | 284 | 31.927 | -14.166 | 30.499 | 1.00 | 42.01 | BLGL |
| ATOM | 2128 | C | GLY | 284 | 30.920 | -13.195 | 29.918 | 1.00 | 40.47 | BLGL |
| ATOM | 2129 | O | GLY | 284 | 30.072 | -13.590 | 29.114 | 1.00 | 41.73 | BLGL |
| ATOM | 2130 | N | GLN | 285 | 30.997 | -11.929 | 30.321 | 1.00 | 36.97 | BLGL |
| ATOM | 2131 | CA | GLN | 285 | 30.081 | -10.934 | 29.794 | 1.00 | 32.62 | BLGL |
| ATOM | 2132 | CB | GLN | 285 | 29.904 | -9.781 | 30.771 | 1.00 | 31.11 | BLGL |
| ATOM | 2133 | CG | GLN | 285 | 29.440 | -10.187 | 32.149 | 1.00 | 29.26 | BLGL |
| ATOM | 2134 | CD | GLN | 285 | 29.234 | -8.985 | 33.046 | 1.00 | 27.08 | BLGL |
| ATOM | 2135 | OE1 | GLN | 285 | 29.922 | -7.973 | 32.910 | 1.00 | 26.10 | BLGL |
| ATOM | 2136 | NE2 | GLN | 285 | 28.296 | -9.091 | 33.974 | 1.00 | 25.79 | BLGL |
| ATOM | 2137 | C | GLN | 285 | 30.634 | -10.397 | 28.487 | 1.00 | 30.85 | BLGL |
| ATOM | 2138 | O | GLN | 285 | 31.844 | -10.301 | 28.302 | 1.00 | 31.43 | BLGL |
| ATOM | 2139 | N | THR | 286 | 29.735 | -10.047 | 27.581 | 1.00 | 29.00 | BLGL |
| ATOM | 2140 | CA | THR | 286 | 30.119 | -9.516 | 26.292 | 1.00 | 26.23 | BLGL |
| ATOM | 2141 | CB | THR | 286 | 29.000 | -9.741 | 25.280 | 1.00 | 26.60 | BLGL |
| ATOM | 2142 | OG1 | THR | 286 | 28.755 | -11.147 | 25.159 | 1.00 | 26.51 | BLGL |
| ATOM | 2143 | CG2 | THR | 286 | 29.370 | -9.150 | 23.928 | 1.00 | 26.18 | BLGL |
| ATOM | 2144 | C | THR | 286 | 30.401 | -8.030 | 26.413 | 1.00 | 25.38 | BLGL |
| ATOM | 2145 | O | THR | 286 | 29.553 | -7.266 | 26.859 | 1.00 | 25.73 | BLGL |
| ATOM | 2146 | N | LEU | 287 | 31.596 | -7.619 | 26.016 | 1.00 | 25.58 | BLGL |
| ATOM | 2147 | CA | LEU | 287 | 31.957 | -6.219 | 26.098 | 1.00 | 25.95 | BLGL |
| ATOM | 2148 | CB | LEU | 287 | 33.036 | -6.034 | 27.159 | 1.00 | 23.53 | BLGL |
| ATOM | 2149 | CG | LEU | 287 | 32.593 | -6.516 | 28.539 | 1.00 | 22.29 | BLGL |
| ATOM | 2150 | CD1 | LEU | 287 | 33.742 | -6.413 | 29.523 | 1.00 | 21.57 | BLGL |
| ATOM | 2151 | CD2 | LEU | 287 | 31.409 | -5.692 | 28.998 | 1.00 | 20.26 | BLGL |
| ATOM | 2152 | C | LEU | 287 | 32.446 | -5.739 | 24.748 | 1.00 | 28.08 | BLGL |
| ATOM | 2153 | O | LEU | 287 | 33.648 | -5.666 | 24.503 | 1.00 | 29.85 | BLGL |
| ATOM | 2154 | N | ASN | 288 | 31.508 | -5.406 | 23.870 | 1.00 | 29.45 | BLGL |
| ATOM | 2155 | CA | ASN | 288 | 31.869 | -4.949 | 22.537 | 1.00 | 31.56 | BLGL |
| ATOM | 2156 | CB | ASN | 288 | 30.641 | -4.928 | 21.632 | 1.00 | 35.67 | BLGL |
| ATOM | 2157 | CG | ASN | 288 | 30.039 | -6.306 | 21.456 | 1.00 | 41.56 | BLGL |
| ATOM | 2158 | OD1 | ASN | 288 | 30.766 | -7.298 | 21.320 | 1.00 | 42.80 | BLGL |
| ATOM | 2159 | ND2 | ASN | 288 | 28.707 | -6.380 | 21.449 | 1.00 | 43.66 | BLGL |
| ATOM | 2160 | C | ASN | 288 | 32.533 | -3.590 | 22.523 | 1.00 | 30.88 | BLGL |
| ATOM | 2161 | O | ASN | 288 | 33.295 | -3.281 | 21.615 | 1.00 | 32.37 | BLGL |
| ATOM | 2162 | N | ASN | 289 | 32.242 | -2.767 | 23.520 | 1.00 | 30.69 | BLGL |
| ATOM | 2163 | CA | ASN | 289 | 32.849 | -1.447 | 23.583 | 1.00 | 29.17 | BLGL |
| ATOM | 2164 | CB | ASN | 289 | 31.778 | -0.364 | 23.737 | 1.00 | 29.80 | BLGL |
| ATOM | 2165 | CG | ASN | 289 | 31.108 | -0.018 | 22.420 | 1.00 | 34.65 | BLGL |
| ATOM | 2166 | OD1 | ASN | 289 | 31.733 | 0.562 | 21.529 | 1.00 | 36.80 | BLGL |
| ATOM | 2167 | ND2 | ASN | 289 | 29.834 | -0.382 | 22.285 | 1.00 | 34.27 | BLGL |
| ATOM | 2168 | C | ASN | 289 | 33.818 | -1.386 | 24.746 | 1.00 | 28.28 | BLGL |
| ATOM | 2169 | O | ASN | 289 | 33.698 | -2.144 | 25.718 | 1.00 | 26.00 | BLGL |
| ATOM | 2170 | N | PRO | 290 | 34.815 | -0.497 | 24.654 | 1.00 | 26.69 | BLGL |
| ATOM | 2171 | CD | PRO | 290 | 35.116 | 0.459 | 23.576 | 1.00 | 25.39 | BLGL |
| ATOM | 2172 | CA | PRO | 290 | 35.783 | -0.375 | 25.740 | 1.00 | 24.60 | BLGL |
| ATOM | 2173 | CB | PRO | 290 | 36.796 | 0.616 | 25.184 | 1.00 | 23.11 | BLGL |
| ATOM | 2174 | CG | PRO | 290 | 35.977 | 1.470 | 24.294 | 1.00 | 24.06 | BLGL |
| ATOM | 2175 | C | PRO | 290 | 35.098 | 0.132 | 27.006 | 1.00 | 25.03 | BLGL |
| ATOM | 2176 | O | PRO | 290 | 34.140 | 0.916 | 26.951 | 1.00 | 24.16 | BLGL |
| ATOM | 2177 | N | VAL | 291 | 35.582 | -0.334 | 28.149 | 1.00 | 23.84 | BLGL |

# Fig. 4 cont.

| ATOM | 2178 | CA | VAL | 291 | 35.019 | 0.083 | 29.420 | 1.00 | 21.28 | BLGL |
|------|------|----|----|----|--------|-------|--------|------|-------|------|
| ATOM | 2179 | CB | VAL | 291 | 35.340 | -0.945 | 30.520 | 1.00 | 21.94 | BLGL |
| ATOM | 2180 | CG1 | VAL | 291 | 34.752 | -0.488 | 31.852 | 1.00 | 20.42 | BLGL |
| ATOM | 2181 | CG2 | VAL | 291 | 34.775 | -2.309 | 30.114 | 1.00 | 17.11 | BLGL |
| ATOM | 2182 | C | VAL | 291 | 35.607 | 1.448 | 29.760 | 1.00 | 20.16 | BLGL |
| ATOM | 2183 | O | VAL | 291 | 36.504 | 1.574 | 30.588 | 1.00 | 19.20 | BLGL |
| ATOM | 2184 | N | THR | 292 | 35.100 | 2.464 | 29.070 | 1.00 | 19.49 | BLGL |
| ATOM | 2185 | CA | THR | 292 | 35.532 | 3.842 | 29.250 | 1.00 | 18.74 | BLGL |
| ATOM | 2186 | CB | THR | 292 | 36.660 | 4.228 | 28.251 | 1.00 | 18.53 | BLGL |
| ATOM | 2187 | OG1 | THR | 292 | 36.111 | 4.400 | 26.939 | 1.00 | 17.67 | BLGL |
| ATOM | 2188 | CG2 | THR | 292 | 37.716 | 3.148 | 28.196 | 1.00 | 17.15 | BLGL |
| ATOM | 2189 | C | THR | 292 | 34.335 | 4.759 | 28.994 | 1.00 | 19.39 | BLGL |
| ATOM | 2190 | O | THR | 292 | 33.275 | 4.308 | 28.568 | 1.00 | 19.27 | BLGL |
| ATOM | 2191 | N | VAL | 293 | 34.514 | 6.048 | 29.252 | 1.00 | 20.06 | BLGL |
| ATOM | 2192 | CA | VAL | 293 | 33.446 | 7.005 | 29.039 | 1.00 | 20.55 | BLGL |
| ATOM | 2193 | CB | VAL | 293 | 33.865 | 8.406 | 29.544 | 1.00 | 20.16 | BLGL |
| ATOM | 2194 | CG1 | VAL | 293 | 32.857 | 9.451 | 29.100 | 1.00 | 20.66 | BLGL |
| ATOM | 2195 | CG2 | VAL | 293 | 33.936 | 8.390 | 31.074 | 1.00 | 16.78 | BLGL |
| ATOM | 2196 | C | VAL | 293 | 33.051 | 7.044 | 27.562 | 1.00 | 20.97 | BLGL |
| ATOM | 2197 | O | VAL | 293 | 31.864 | 7.124 | 27.234 | 1.00 | 21.53 | BLGL |
| ATOM | 2198 | N | GLN | 294 | 34.039 | 6.962 | 26.674 | 1.00 | 20.45 | BLGL |
| ATOM | 2199 | CA | GLN | 294 | 33.770 | 6.956 | 25.238 | 1.00 | 21.64 | BLGL |
| ATOM | 2200 | CB | GLN | 294 | 35.066 | 7.058 | 24.431 | 1.00 | 25.60 | BLGL |
| ATOM | 2201 | CG | GLN | 294 | 35.192 | 8.341 | 23.619 | 1.00 | 29.52 | BLGL |
| ATOM | 2202 | CD | GLN | 294 | 34.031 | 8.562 | 22.666 | 1.00 | 29.94 | BLGL |
| ATOM | 2203 | OE1 | GLN | 294 | 33.739 | 9.696 | 22.296 | 1.00 | 34.05 | BLGL |
| ATOM | 2204 | NE2 | GLN | 294 | 33.371 | 7.485 | 22.260 | 1.00 | 28.56 | BLGL |
| ATOM | 2205 | C | GLN | 294 | 33.058 | 5.672 | 24.834 | 1.00 | 22.39 | BLGL |
| ATOM | 2206 | O | GLN | 294 | 32.199 | 5.677 | 23.950 | 1.00 | 19.94 | BLGL |
| ATOM | 2207 | N | GLY | 295 | 33.444 | 4.566 | 25.468 | 1.00 | 22.59 | BLGL |
| ATOM | 2208 | CA | GLY | 295 | 32.814 | 3.295 | 25.173 | 1.00 | 20.59 | BLGL |
| ATOM | 2209 | C | GLY | 295 | 31.349 | 3.362 | 25.564 | 1.00 | 22.43 | BLGL |
| ATOM | 2210 | O | GLY | 295 | 30.464 | 3.047 | 24.767 | 1.00 | 23.22 | BLGL |
| ATOM | 2211 | N | GLN | 296 | 31.099 | 3.787 | 26.798 | 1.00 | 19.02 | BLGL |
| ATOM | 2212 | CA | GLN | 296 | 29.750 | 3.905 | 27.313 | 1.00 | 19.21 | BLGL |
| ATOM | 2213 | CB | GLN | 296 | 29.789 | 4.581 | 28.683 | 1.00 | 19.90 | BLGL |
| ATOM | 2214 | CG | GLN | 296 | 28.467 | 4.668 | 29.419 | 1.00 | 18.48 | BLGL |
| ATOM | 2215 | CD | GLN | 296 | 28.572 | 5.536 | 30.669 | 1.00 | 17.80 | BLGL |
| ATOM | 2216 | OE1 | GLN | 296 | 29.027 | 6.679 | 30.595 | 1.00 | 16.03 | BLGL |
| ATOM | 2217 | NE2 | GLN | 296 | 28.152 | 4.999 | 31.818 | 1.00 | 15.03 | BLGL |
| ATOM | 2218 | C | GLN | 296 | 28.906 | 4.719 | 26.336 | 1.00 | 19.79 | BLGL |
| ATOM | 2219 | O | GLN | 296 | 27.777 | 4.347 | 26.016 | 1.00 | 20.36 | BLGL |
| ATOM | 2220 | N | ALA | 297 | 29.458 | 5.825 | 25.851 | 1.00 | 18.99 | BLGL |
| ATOM | 2221 | CA | ALA | 297 | 28.733 | 6.669 | 24.905 | 1.00 | 18.45 | BLGL |
| ATOM | 2222 | CB | ALA | 297 | 29.546 | 7.916 | 24.578 | 1.00 | 14.36 | BLGL |
| ATOM | 2223 | C | ALA | 297 | 28.416 | 5.895 | 23.630 | 1.00 | 19.50 | BLGL |
| ATOM | 2224 | O | ALA | 297 | 27.301 | 5.978 | 23.104 | 1.00 | 20.34 | BLGL |
| ATOM | 2225 | N | ASN | 298 | 29.395 | 5.142 | 23.135 | 1.00 | 19.83 | BLGL |
| ATOM | 2226 | CA | ASN | 298 | 29.196 | 4.352 | 21.926 | 1.00 | 21.45 | BLGL |
| ATOM | 2227 | CB | ASN | 298 | 30.442 | 3.524 | 21.592 | 1.00 | 24.97 | BLGL |
| ATOM | 2228 | CG | ASN | 298 | 31.563 | 4.358 | 20.999 | 1.00 | 26.63 | BLGL |
| ATOM | 2229 | OD1 | ASN | 298 | 31.329 | 5.440 | 20.459 | 1.00 | 25.65 | BLGL |
| ATOM | 2230 | ND2 | ASN | 298 | 32.791 | 3.843 | 21.078 | 1.00 | 27.74 | BLGL |
| ATOM | 2231 | C | ASN | 298 | 28.027 | 3.405 | 22.133 | 1.00 | 21.39 | BLGL |
| ATOM | 2232 | O | ASN | 298 | 27.130 | 3.306 | 21.297 | 1.00 | 21.38 | BLGL |
| ATOM | 2233 | N | ALA | 299 | 28.061 | 2.713 | 23.266 | 1.00 | 19.25 | BLGL |
| ATOM | 2234 | CA | ALA | 299 | 27.038 | 1.754 | 23.633 | 1.00 | 17.97 | BLGL |
| ATOM | 2235 | CB | ALA | 299 | 27.294 | 1.264 | 25.030 | 1.00 | 16.35 | BLGL |
| ATOM | 2236 | C | ALA | 299 | 25.638 | 2.339 | 23.537 | 1.00 | 19.35 | BLGL |
| ATOM | 2237 | O | ALA | 299 | 24.763 | 1.771 | 22.881 | 1.00 | 17.73 | BLGL |
| ATOM | 2238 | N | VAL | 300 | 25.432 | 3.474 | 24.201 | 1.00 | 20.77 | BLGL |
| ATOM | 2239 | CA | VAL | 300 | 24.134 | 4.146 | 24.202 | 1.00 | 20.54 | BLGL |
| ATOM | 2240 | CB | VAL | 300 | 24.141 | 5.382 | 25.141 | 1.00 | 19.20 | BLGL |
| ATOM | 2241 | CG1 | VAL | 300 | 22.786 | 6.081 | 25.108 | 1.00 | 16.54 | BLGL |
| ATOM | 2242 | CG2 | VAL | 300 | 24.467 | 4.948 | 26.556 | 1.00 | 16.81 | BLGL |
| ATOM | 2243 | C | VAL | 300 | 23.761 | 4.597 | 22.795 | 1.00 | 20.62 | BLGL |

# Fig. 4 cont.

| ATOM | 2244 | O   | VAL | 300 | 22.643 | 4.383  | 22.332 | 1.00 | 22.02 | BLGL |
|------|------|-----|-----|-----|--------|--------|--------|------|-------|------|
| ATOM | 2245 | N   | ARG | 301 | 24.711 | 5.220  | 22.117 | 1.00 | 19.80 | BLGL |
| ATOM | 2246 | CA  | ARG | 301 | 24.485 | 5.699  | 20.770 | 1.00 | 20.87 | BLGL |
| ATOM | 2247 | CB  | ARG | 301 | 25.764 | 6.370  | 20.273 | 1.00 | 20.72 | BLGL |
| ATOM | 2248 | CG  | ARG | 301 | 25.697 | 6.960  | 18.884 | 1.00 | 19.75 | BLGL |
| ATOM | 2249 | CD  | ARG | 301 | 25.963 | 5.909  | 17.841 | 1.00 | 20.20 | BLGL |
| ATOM | 2250 | NE  | ARG | 301 | 25.950 | 6.479  | 16.502 | 1.00 | 21.66 | BLGL |
| ATOM | 2251 | CZ  | ARG | 301 | 25.770 | 5.763  | 15.400 | 1.00 | 21.05 | BLGL |
| ATOM | 2252 | NH1 | ARG | 301 | 25.593 | 4.453  | 15.484 | 1.00 | 23.39 | BLGL |
| ATOM | 2253 | NH2 | ARG | 301 | 25.741 | 6.359  | 14.223 | 1.00 | 19.98 | BLGL |
| ATOM | 2254 | C   | ARG | 301 | 24.050 | 4.575  | 19.824 | 1.00 | 21.51 | BLGL |
| ATOM | 2255 | O   | ARG | 301 | 23.190 | 4.774  | 18.967 | 1.00 | 23.05 | BLGL |
| ATOM | 2256 | N   | ASP | 302 | 24.633 | 3.394  | 19.989 | 1.00 | 20.34 | BLGL |
| ATOM | 2257 | CA  | ASP | 302 | 24.306 | 2.262  | 19.138 | 1.00 | 19.74 | BLGL |
| ATOM | 2258 | CB  | ASP | 302 | 25.378 | 1.190  | 19.260 | 1.00 | 22.07 | BLGL |
| ATOM | 2259 | CG  | ASP | 302 | 26.659 | 1.571  | 18.548 | 1.00 | 26.74 | BLGL |
| ATOM | 2260 | OD1 | ASP | 302 | 27.647 | 0.818  | 18.676 | 1.00 | 31.70 | BLGL |
| ATOM | 2261 | OD2 | ASP | 302 | 26.686 | 2.618  | 17.857 | 1.00 | 28.72 | BLGL |
| ATOM | 2262 | C   | ASP | 302 | 22.947 | 1.648  | 19.408 | 1.00 | 20.74 | BLGL |
| ATOM | 2263 | O   | ASP | 302 | 22.329 | 1.083  | 18.509 | 1.00 | 23.13 | BLGL |
| ATOM | 2264 | N   | VAL | 303 | 22.482 | 1.740  | 20.644 | 1.00 | 18.00 | BLGL |
| ATOM | 2265 | CA  | VAL | 303 | 21.182 | 1.189  | 20.971 | 1.00 | 18.00 | BLGL |
| ATOM | 2266 | CB  | VAL | 303 | 20.971 | 1.110  | 22.503 | 1.00 | 17.67 | BLGL |
| ATOM | 2267 | CG1 | VAL | 303 | 19.626 | 0.483  | 22.813 | 1.00 | 17.30 | BLGL |
| ATOM | 2268 | CG2 | VAL | 303 | 22.075 | 0.299  | 23.132 | 1.00 | 20.13 | BLGL |
| ATOM | 2269 | C   | VAL | 303 | 20.126 | 2.099  | 20.346 | 1.00 | 18.76 | BLGL |
| ATOM | 2270 | O   | VAL | 303 | 19.099 | 1.638  | 19.854 | 1.00 | 16.54 | BLGL |
| ATOM | 2271 | N   | ILE | 304 | 20.392 | 3.401  | 20.367 | 1.00 | 19.37 | BLGL |
| ATOM | 2272 | CA  | ILE | 304 | 19.471 | 4.371  | 19.793 | 1.00 | 20.60 | BLGL |
| ATOM | 2273 | CB  | ILE | 304 | 19.955 | 5.820  | 20.067 | 1.00 | 21.68 | BLGL |
| ATOM | 2274 | CG2 | ILE | 304 | 19.113 | 6.835  | 19.293 | 1.00 | 19.25 | BLGL |
| ATOM | 2275 | CG1 | ILE | 304 | 19.853 | 6.108  | 21.567 | 1.00 | 21.33 | BLGL |
| ATOM | 2276 | CD1 | ILE | 304 | 20.334 | 7.482  | 21.961 | 1.00 | 21.10 | BLGL |
| ATOM | 2277 | C   | ILE | 304 | 19.387 | 4.102  | 18.294 | 1.00 | 21.62 | BLGL |
| ATOM | 2278 | O   | ILE | 304 | 18.316 | 4.130  | 17.695 | 1.00 | 22.05 | BLGL |
| ATOM | 2279 | N   | GLN | 305 | 20.531 | 3.820  | 17.694 | 1.00 | 21.95 | BLGL |
| ATOM | 2280 | CA  | GLN | 305 | 20.579 | 3.523  | 16.279 | 1.00 | 22.70 | BLGL |
| ATOM | 2281 | CB  | GLN | 305 | 22.031 | 3.274  | 15.855 | 1.00 | 25.34 | BLGL |
| ATOM | 2282 | CG  | GLN | 305 | 22.203 | 2.958  | 14.381 | 1.00 | 28.30 | BLGL |
| ATOM | 2283 | CD  | GLN | 305 | 22.031 | 4.178  | 13.505 | 1.00 | 30.27 | BLGL |
| ATOM | 2284 | OE1 | GLN | 305 | 22.915 | 5.030  | 13.430 | 1.00 | 30.12 | BLGL |
| ATOM | 2285 | NE2 | GLN | 305 | 20.884 | 4.273  | 12.841 | 1.00 | 32.34 | BLGL |
| ATOM | 2286 | C   | GLN | 305 | 19.736 | 2.278  | 16.006 | 1.00 | 22.92 | BLGL |
| ATOM | 2287 | O   | GLN | 305 | 18.925 | 2.258  | 15.080 | 1.00 | 23.46 | BLGL |
| ATOM | 2288 | N   | ALA | 306 | 19.931 | 1.247  | 16.831 | 1.00 | 22.84 | BLGL |
| ATOM | 2289 | CA  | ALA | 306 | 19.221 | -0.031 | 16.693 | 1.00 | 21.78 | BLGL |
| ATOM | 2290 | CB  | ALA | 306 | 19.708 | -1.019 | 17.743 | 1.00 | 18.27 | BLGL |
| ATOM | 2291 | C   | ALA | 306 | 17.704 | 0.090  | 16.773 | 1.00 | 22.33 | BLGL |
| ATOM | 2292 | O   | ALA | 306 | 16.987 | -0.569 | 16.018 | 1.00 | 23.37 | BLGL |
| ATOM | 2293 | N   | VAL | 307 | 17.219 | 0.919  | 17.691 | 1.00 | 20.00 | BLGL |
| ATOM | 2294 | CA  | VAL | 307 | 15.788 | 1.112  | 17.844 | 1.00 | 20.55 | BLGL |
| ATOM | 2295 | CB  | VAL | 307 | 15.450 | 1.823  | 19.169 | 1.00 | 20.50 | BLGL |
| ATOM | 2296 | CG1 | VAL | 307 | 13.959 | 2.106  | 19.248 | 1.00 | 17.36 | BLGL |
| ATOM | 2297 | CG2 | VAL | 307 | 15.878 | 0.960  | 20.337 | 1.00 | 19.55 | BLGL |
| ATOM | 2298 | C   | VAL | 307 | 15.274 | 1.959  | 16.696 | 1.00 | 21.97 | BLGL |
| ATOM | 2299 | O   | VAL | 307 | 14.164 | 1.750  | 16.195 | 1.00 | 22.69 | BLGL |
| ATOM | 2300 | N   | SER | 308 | 16.097 | 2.916  | 16.283 | 1.00 | 21.64 | BLGL |
| ATOM | 2301 | CA  | SER | 308 | 15.750 | 3.818  | 15.197 | 1.00 | 21.48 | BLGL |
| ATOM | 2302 | CB  | SER | 308 | 16.809 | 4.916  | 15.073 | 1.00 | 22.23 | BLGL |
| ATOM | 2303 | OG  | SER | 308 | 16.510 | 5.812  | 14.018 | 1.00 | 26.06 | BLGL |
| ATOM | 2304 | C   | SER | 308 | 15.633 | 3.059  | 13.885 | 1.00 | 20.97 | BLGL |
| ATOM | 2305 | O   | SER | 308 | 14.781 | 3.372  | 13.054 | 1.00 | 17.14 | BLGL |
| ATOM | 2306 | N   | ASP | 309 | 16.490 | 2.057  | 13.709 | 1.00 | 21.61 | BLGL |
| ATOM | 2307 | CA  | ASP | 309 | 16.480 | 1.252  | 12.494 | 1.00 | 23.50 | BLGL |
| ATOM | 2308 | CB  | ASP | 309 | 17.698 | 0.332  | 12.434 | 1.00 | 25.27 | BLGL |
| ATOM | 2309 | CG  | ASP | 309 | 18.971 | 1.069  | 12.064 | 1.00 | 29.05 | BLGL |

# Fig. 4 cont.

| ATOM | 2310 | OD1 | ASP | 309 | 18.874 | 2.130 | 11.401 | 1.00 | 26.38 | BLGL |
|------|------|-----|-----|-----|--------|-------|--------|------|-------|------|
| ATOM | 2311 | OD2 | ASP | 309 | 20.066 | 0.576 | 12.423 | 1.00 | 30.01 | BLGL |
| ATOM | 2312 | C | ASP | 309 | 15.225 | 0.412 | 12.339 | 1.00 | 24.33 | BLGL |
| ATOM | 2313 | O | ASP | 309 | 14.972 | -0.124 | 11.265 | 1.00 | 26.71 | BLGL |
| ATOM | 2314 | N | VAL | 310 | 14.450 | 0.280 | 13.409 | 1.00 | 24.29 | BLGL |
| ATOM | 2315 | CA | VAL | 310 | 13.219 | -0.490 | 13.344 | 1.00 | 23.62 | BLGL |
| ATOM | 2316 | CB | VAL | 310 | 12.582 | -0.647 | 14.730 | 1.00 | 23.06 | BLGL |
| ATOM | 2317 | CG1 | VAL | 310 | 11.232 | -1.336 | 14.606 | 1.00 | 21.23 | BLGL |
| ATOM | 2318 | CG2 | VAL | 310 | 13.509 | -1.443 | 15.632 | 1.00 | 21.91 | BLGL |
| ATOM | 2319 | C | VAL | 310 | 12.248 | 0.247 | 12.440 | 1.00 | 23.63 | BLGL |
| ATOM | 2320 | O | VAL | 310 | 11.360 | -0.352 | 11.834 | 1.00 | 25.38 | BLGL |
| ATOM | 2321 | N | GLY | 311 | 12.438 | 1.555 | 12.343 | 1.00 | 23.71 | BLGL |
| ATOM | 2322 | CA | GLY | 311 | 11.573 | 2.373 | 11.519 | 1.00 | 23.98 | BLGL |
| ATOM | 2323 | C | GLY | 311 | 10.628 | 3.201 | 12.366 | 1.00 | 27.47 | BLGL |
| ATOM | 2324 | O | GLY | 311 | 10.919 | 3.565 | 13.514 | 1.00 | 28.40 | BLGL |
| ATOM | 2325 | N | GLU | 312 | 9.469 | 3.474 | 11.783 | 1.00 | 27.49 | BLGL |
| ATOM | 2326 | CA | GLU | 312 | 8.438 | 4.262 | 12.419 | 1.00 | 27.36 | BLGL |
| ATOM | 2327 | CB | GLU | 312 | 7.210 | 4.291 | 11.514 | 1.00 | 32.86 | BLGL |
| ATOM | 2328 | CG | GLU | 312 | 6.318 | 5.503 | 11.705 | 1.00 | 43.92 | BLGL |
| ATOM | 2329 | CD | GLU | 312 | 4.950 | 5.314 | 11.071 | 1.00 | 50.44 | BLGL |
| ATOM | 2330 | OE1 | GLU | 312 | 4.889 | 4.793 | 9.930 | 1.00 | 51.60 | BLGL |
| ATOM | 2331 | OE2 | GLU | 312 | 3.939 | 5.694 | 11.713 | 1.00 | 53.86 | BLGL |
| ATOM | 2332 | C | GLU | 312 | 8.039 | 3.746 | 13.805 | 1.00 | 25.87 | BLGL |
| ATOM | 2333 | O | GLU | 312 | 7.717 | 4.537 | 14.683 | 1.00 | 27.15 | BLGL |
| ATOM | 2334 | N | ALA | 313 | 8.067 | 2.431 | 14.003 | 1.00 | 22.50 | BLGL |
| ATOM | 2335 | CA | ALA | 313 | 7.671 | 1.814 | 15.273 | 1.00 | 19.75 | BLGL |
| ATOM | 2336 | CB | ALA | 313 | 7.480 | 0.315 | 15.077 | 1.00 | 19.28 | BLGL |
| ATOM | 2337 | C | ALA | 313 | 8.608 | 2.054 | 16.454 | 1.00 | 18.86 | BLGL |
| ATOM | 2338 | O | ALA | 313 | 8.167 | 2.049 | 17.602 | 1.00 | 15.56 | BLGL |
| ATOM | 2339 | N | GLY | 314 | 9.897 | 2.238 | 16.173 | 1.00 | 19.40 | BLGL |
| ATOM | 2340 | CA | GLY | 314 | 10.868 | 2.476 | 17.232 | 1.00 | 21.12 | BLGL |
| ATOM | 2341 | C | GLY | 314 | 10.667 | 3.878 | 17.787 | 1.00 | 22.30 | BLGL |
| ATOM | 2342 | O | GLY | 314 | 11.016 | 4.865 | 17.135 | 1.00 | 23.19 | BLGL |
| ATOM | 2343 | N | ILE | 315 | 10.122 | 3.973 | 18.997 | 1.00 | 19.98 | BLGL |
| ATOM | 2344 | CA | ILE | 315 | 9.841 | 5.267 | 19.580 | 1.00 | 18.06 | BLGL |
| ATOM | 2345 | CB | ILE | 315 | 8.457 | 5.265 | 20.248 | 1.00 | 17.92 | BLGL |
| ATOM | 2346 | CG2 | ILE | 315 | 7.402 | 4.928 | 19.221 | 1.00 | 16.03 | BLGL |
| ATOM | 2347 | CG1 | ILE | 315 | 8.417 | 4.242 | 21.378 | 1.00 | 17.81 | BLGL |
| ATOM | 2348 | CD1 | ILE | 315 | 7.113 | 4.236 | 22.116 | 1.00 | 16.57 | BLGL |
| ATOM | 2349 | C | ILE | 315 | 10.852 | 5.818 | 20.563 | 1.00 | 18.49 | BLGL |
| ATOM | 2350 | O | ILE | 315 | 10.851 | 7.012 | 20.836 | 1.00 | 19.85 | BLGL |
| ATOM | 2351 | N | GLY | 316 | 11.719 | 4.974 | 21.101 | 1.00 | 18.64 | BLGL |
| ATOM | 2352 | CA | GLY | 316 | 12.692 | 5.492 | 22.042 | 1.00 | 17.78 | BLGL |
| ATOM | 2353 | C | GLY | 316 | 13.562 | 4.510 | 22.803 | 1.00 | 18.38 | BLGL |
| ATOM | 2354 | O | GLY | 316 | 13.500 | 3.290 | 22.618 | 1.00 | 17.99 | BLGL |
| ATOM | 2355 | N | VAL | 317 | 14.381 | 5.081 | 23.680 | 1.00 | 17.69 | BLGL |
| ATOM | 2356 | CA | VAL | 317 | 15.312 | 4.328 | 24.512 | 1.00 | 17.45 | BLGL |
| ATOM | 2357 | CB | VAL | 317 | 16.727 | 4.367 | 23.916 | 1.00 | 17.12 | BLGL |
| ATOM | 2358 | CG1 | VAL | 317 | 17.710 | 3.738 | 24.882 | 1.00 | 16.69 | BLGL |
| ATOM | 2359 | CG2 | VAL | 317 | 16.753 | 3.642 | 22.586 | 1.00 | 16.13 | BLGL |
| ATOM | 2360 | C | VAL | 317 | 15.385 | 4.902 | 25.921 | 1.00 | 17.08 | BLGL |
| ATOM | 2361 | O | VAL | 317 | 15.386 | 6.116 | 26.101 | 1.00 | 19.09 | BLGL |
| ATOM | 2362 | N | PHE | 318 | 15.441 | 4.032 | 26.920 | 1.00 | 17.11 | BLGL |
| ATOM | 2363 | CA | PHE | 318 | 15.547 | 4.488 | 28.298 | 1.00 | 16.85 | BLGL |
| ATOM | 2364 | CB | PHE | 318 | 14.389 | 3.976 | 29.146 | 1.00 | 17.66 | BLGL |
| ATOM | 2365 | CG | PHE | 318 | 13.154 | 4.821 | 29.068 | 1.00 | 19.59 | BLGL |
| ATOM | 2366 | CD1 | PHE | 318 | 12.208 | 4.615 | 28.063 | 1.00 | 17.88 | BLGL |
| ATOM | 2367 | CD2 | PHE | 318 | 12.922 | 5.811 | 30.017 | 1.00 | 18.14 | BLGL |
| ATOM | 2368 | CE1 | PHE | 318 | 11.041 | 5.383 | 28.007 | 1.00 | 15.40 | BLGL |
| ATOM | 2369 | CE2 | PHE | 318 | 11.760 | 6.585 | 29.968 | 1.00 | 20.01 | BLGL |
| ATOM | 2370 | CZ | PHE | 318 | 10.815 | 6.367 | 28.960 | 1.00 | 16.53 | BLGL |
| ATOM | 2371 | C | PHE | 318 | 16.839 | 3.996 | 28.914 | 1.00 | 17.63 | BLGL |
| ATOM | 2372 | O | PHE | 318 | 17.132 | 2.802 | 28.878 | 1.00 | 19.56 | BLGL |
| ATOM | 2373 | N | TYR | 319 | 17.619 | 4.914 | 29.471 | 1.00 | 17.12 | BLGL |
| ATOM | 2374 | CA | TYR | 319 | 18.859 | 4.531 | 30.127 | 1.00 | 17.31 | BLGL |
| ATOM | 2375 | CB | TYR | 319 | 19.876 | 5.676 | 30.103 | 1.00 | 15.56 | BLGL |

# Fig. 4 cont.

| ATOM | 2376 | CG | TYR | 319 | 21.255 | 5.211 | 30.495 | 1.00 | 17.60 | BLGL |
|------|------|-----|-----|-----|--------|--------|--------|------|-------|------|
| ATOM | 2377 | CD1 | TYR | 319 | 22.257 | 5.060 | 29.541 | 1.00 | 16.51 | BLGL |
| ATOM | 2378 | CE1 | TYR | 319 | 23.503 | 4.568 | 29.886 | 1.00 | 17.94 | BLGL |
| ATOM | 2379 | CD2 | TYR | 319 | 21.541 | 4.860 | 31.815 | 1.00 | 17.35 | BLGL |
| ATOM | 2380 | CE2 | TYR | 319 | 22.781 | 4.366 | 32.174 | 1.00 | 18.20 | BLGL |
| ATOM | 2381 | CZ | TYR | 319 | 23.761 | 4.220 | 31.207 | 1.00 | 18.82 | BLGL |
| ATOM | 2382 | OH | TYR | 319 | 24.993 | 3.717 | 31.560 | 1.00 | 17.43 | BLGL |
| ATOM | 2383 | C | TYR | 319 | 18.465 | 4.214 | 31.568 | 1.00 | 15.84 | BLGL |
| ATOM | 2384 | O | TYR | 319 | 17.852 | 5.040 | 32.231 | 1.00 | 17.43 | BLGL |
| ATOM | 2385 | N | TRP | 320 | 18.811 | 3.024 | 32.050 | 1.00 | 15.86 | BLGL |
| ATOM | 2386 | CA | TRP | 320 | 18.448 | 2.622 | 33.408 | 1.00 | 14.37 | BLGL |
| ATOM | 2387 | CB | TRP | 320 | 18.286 | 1.099 | 33.489 | 1.00 | 13.03 | BLGL |
| ATOM | 2388 | CG | TRP | 320 | 17.673 | 0.644 | 34.786 | 1.00 | 13.67 | BLGL |
| ATOM | 2389 | CD2 | TRP | 320 | 18.348 | -0.001 | 35.873 | 1.00 | 13.63 | BLGL |
| ATOM | 2390 | CE2 | TRP | 320 | 17.408 | -0.123 | 36.930 | 1.00 | 16.14 | BLGL |
| ATOM | 2391 | CE3 | TRP | 320 | 19.654 | -0.480 | 36.063 | 1.00 | 12.95 | BLGL |
| ATOM | 2392 | CD1 | TRP | 320 | 16.388 | 0.865 | 35.210 | 1.00 | 10.20 | BLGL |
| ATOM | 2393 | NE1 | TRP | 320 | 16.225 | 0.413 | 36.491 | 1.00 | 11.94 | BLGL |
| ATOM | 2394 | CZ2 | TRP | 320 | 17.736 | -0.706 | 38.171 | 1.00 | 14.00 | BLGL |
| ATOM | 2395 | CZ3 | TRP | 320 | 19.984 | -1.057 | 37.292 | 1.00 | 14.81 | BLGL |
| ATOM | 2396 | CH2 | TRP | 320 | 19.023 | -1.163 | 38.332 | 1.00 | 15.77 | BLGL |
| ATOM | 2397 | C | TRP | 320 | 19.428 | 3.071 | 34.484 | 1.00 | 14.79 | BLGL |
| ATOM | 2398 | O | TRP | 320 | 20.624 | 2.786 | 34.403 | 1.00 | 13.40 | BLGL |
| ATOM | 2399 | N | GLU | 321 | 18.898 | 3.770 | 35.487 | 1.00 | 14.52 | BLGL |
| ATOM | 2400 | CA | GLU | 321 | 19.671 | 4.261 | 36.630 | 1.00 | 16.07 | BLGL |
| ATOM | 2401 | CB | GLU | 321 | 19.878 | 3.117 | 37.634 | 1.00 | 16.50 | BLGL |
| ATOM | 2402 | CG | GLU | 321 | 18.605 | 2.675 | 38.362 | 1.00 | 15.22 | BLGL |
| ATOM | 2403 | CD | GLU | 321 | 18.179 | 3.653 | 39.439 | 1.00 | 15.33 | BLGL |
| ATOM | 2404 | OE1 | GLU | 321 | 17.190 | 3.375 | 40.156 | 1.00 | 13.74 | BLGL |
| ATOM | 2405 | OE2 | GLU | 321 | 18.840 | 4.703 | 39.573 | 1.00 | 17.28 | BLGL |
| ATOM | 2406 | C | GLU | 321 | 21.015 | 4.890 | 36.267 | 1.00 | 16.30 | BLGL |
| ATOM | 2407 | O | GLU | 321 | 22.078 | 4.321 | 36.533 | 1.00 | 19.88 | BLGL |
| ATOM | 2408 | N | PRO | 322 | 20.985 | 6.085 | 35.664 | 1.00 | 13.95 | BLGL |
| ATOM | 2409 | CD | PRO | 322 | 19.800 | 6.807 | 35.166 | 1.00 | 13.71 | BLGL |
| ATOM | 2410 | CA | PRO | 322 | 22.207 | 6.776 | 35.269 | 1.00 | 13.32 | BLGL |
| ATOM | 2411 | CB | PRO | 322 | 21.727 | 7.665 | 34.136 | 1.00 | 13.68 | BLGL |
| ATOM | 2412 | CG | PRO | 322 | 20.397 | 8.108 | 34.648 | 1.00 | 11.78 | BLGL |
| ATOM | 2413 | C | PRO | 322 | 22.826 | 7.588 | 36.391 | 1.00 | 14.16 | BLGL |
| ATOM | 2414 | O | PRO | 322 | 23.849 | 8.235 | 36.191 | 1.00 | 17.47 | BLGL |
| ATOM | 2415 | N | ALA | 323 | 22.215 | 7.564 | 37.568 | 1.00 | 12.38 | BLGL |
| ATOM | 2416 | CA | ALA | 323 | 22.742 | 8.345 | 38.676 | 1.00 | 11.98 | BLGL |
| ATOM | 2417 | CB | ALA | 323 | 21.979 | 9.660 | 38.786 | 1.00 | 8.04 | BLGL |
| ATOM | 2418 | C | ALA | 323 | 22.736 | 7.619 | 40.012 | 1.00 | 12.24 | BLGL |
| ATOM | 2419 | O | ALA | 323 | 22.580 | 8.245 | 41.060 | 1.00 | 10.55 | BLGL |
| ATOM | 2420 | N | TRP | 324 | 22.910 | 6.300 | 39.980 | 1.00 | 14.35 | BLGL |
| ATOM | 2421 | CA | TRP | 324 | 22.933 | 5.515 | 41.215 | 1.00 | 15.62 | BLGL |
| ATOM | 2422 | CB | TRP | 324 | 22.422 | 4.094 | 40.973 | 1.00 | 15.22 | BLGL |
| ATOM | 2423 | CG | TRP | 324 | 21.843 | 3.473 | 42.201 | 1.00 | 16.28 | BLGL |
| ATOM | 2424 | CD2 | TRP | 324 | 20.827 | 2.465 | 42.257 | 1.00 | 18.02 | BLGL |
| ATOM | 2425 | CE2 | TRP | 324 | 20.595 | 2.181 | 43.622 | 1.00 | 18.70 | BLGL |
| ATOM | 2426 | CE3 | TRP | 324 | 20.086 | 1.776 | 41.287 | 1.00 | 16.37 | BLGL |
| ATOM | 2427 | CD1 | TRP | 324 | 22.178 | 3.748 | 43.494 | 1.00 | 17.37 | BLGL |
| ATOM | 2428 | NE1 | TRP | 324 | 21.434 | 2.978 | 44.354 | 1.00 | 19.41 | BLGL |
| ATOM | 2429 | CZ2 | TRP | 324 | 19.655 | 1.231 | 44.044 | 1.00 | 19.78 | BLGL |
| ATOM | 2430 | CZ3 | TRP | 324 | 19.154 | 0.834 | 41.703 | 1.00 | 16.22 | BLGL |
| ATOM | 2431 | CH2 | TRP | 324 | 18.944 | 0.570 | 43.071 | 1.00 | 18.68 | BLGL |
| ATOM | 2432 | C | TRP | 324 | 24.378 | 5.467 | 41.707 | 1.00 | 16.46 | BLGL |
| ATOM | 2433 | O | TRP | 324 | 24.986 | 4.405 | 41.823 | 1.00 | 13.25 | BLGL |
| ATOM | 2434 | N | ILE | 325 | 24.916 | 6.645 | 41.994 | 1.00 | 18.45 | BLGL |
| ATOM | 2435 | CA | ILE | 325 | 26.284 | 6.781 | 42.453 | 1.00 | 20.02 | BLGL |
| ATOM | 2436 | CB | ILE | 325 | 26.796 | 8.203 | 42.189 | 1.00 | 19.48 | BLGL |
| ATOM | 2437 | CG2 | ILE | 325 | 26.652 | 8.518 | 40.706 | 1.00 | 18.33 | BLGL |
| ATOM | 2438 | CG1 | ILE | 325 | 26.021 | 9.212 | 43.032 | 1.00 | 17.13 | BLGL |
| ATOM | 2439 | CD1 | ILE | 325 | 26.493 | 10.630 | 42.843 | 1.00 | 14.92 | BLGL |
| ATOM | 2440 | C | ILE | 325 | 26.448 | 6.429 | 43.926 | 1.00 | 21.37 | BLGL |
| ATOM | 2441 | O | ILE | 325 | 25.473 | 6.373 | 44.675 | 1.00 | 20.25 | BLGL |

## Fig. 4 cont.

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| ATOM | 2442 | N | PRO | 326 | 27.697 | 6.188 | 44.358 | 1.00 | 22.85 | BLGL |
|------|------|------|-----|-----|--------|-------|--------|------|-------|------|
| ATOM | 2443 | CD | PRO | 326 | 28.935 | 6.258 | 43.557 | 1.00 | 21.92 | BLGL |
| ATOM | 2444 | CA | PRO | 326 | 27.988 | 5.827 | 45.750 | 1.00 | 23.11 | BLGL |
| ATOM | 2445 | CB | PRO | 326 | 29.488 | 5.535 | 45.724 | 1.00 | 21.79 | BLGL |
| ATOM | 2446 | CG | PRO | 326 | 29.992 | 6.401 | 44.613 | 1.00 | 23.00 | BLGL |
| ATOM | 2447 | C | PRO | 326 | 27.604 | 6.851 | 46.806 | 1.00 | 22.87 | BLGL |
| ATOM | 2448 | O | PRO | 326 | 27.666 | 8.055 | 46.564 | 1.00 | 22.51 | BLGL |
| ATOM | 2449 | N | VAL | 327 | 27.189 | 6.360 | 47.975 | 1.00 | 22.78 | BLGL |
| ATOM | 2450 | CA | VAL | 327 | 26.812 | 7.236 | 49.083 | 1.00 | 24.67 | BLGL |
| ATOM | 2451 | CB | VAL | 327 | 25.918 | 6.519 | 50.133 | 1.00 | 26.26 | BLGL |
| ATOM | 2452 | CG1 | VAL | 327 | 24.651 | 5.996 | 49.478 | 1.00 | 27.07 | BLGL |
| ATOM | 2453 | CG2 | VAL | 327 | 26.691 | 5.393 | 50.805 | 1.00 | 23.81 | BLGL |
| ATOM | 2454 | C | VAL | 327 | 28.072 | 7.697 | 49.798 | 1.00 | 25.35 | BLGL |
| ATOM | 2455 | O | VAL | 327 | 28.036 | 8.643 | 50.582 | 1.00 | 25.02 | BLGL |
| ATOM | 2456 | N | GLY | 328 | 29.176 | 7.007 | 49.516 | 1.00 | 26.68 | BLGL |
| ATOM | 2457 | CA | GLY | 328 | 30.459 | 7.315 | 50.120 | 1.00 | 27.54 | BLGL |
| ATOM | 2458 | C | GLY | 328 | 31.540 | 6.412 | 49.551 | 1.00 | 29.31 | BLGL |
| ATOM | 2459 | O | GLY | 328 | 31.219 | 5.392 | 48.938 | 1.00 | 29.16 | BLGL |
| ATOM | 2460 | N | PRO | 329 | 32.830 | 6.751 | 49.743 | 1.00 | 30.18 | BLGL |
| ATOM | 2461 | CD | PRO | 329 | 33.277 | 7.948 | 50.477 | 1.00 | 30.73 | BLGL |
| ATOM | 2462 | CA | PRO | 329 | 33.989 | 5.994 | 49.255 | 1.00 | 30.09 | BLGL |
| ATOM | 2463 | CB | PRO | 329 | 35.166 | 6.722 | 49.891 | 1.00 | 30.88 | BLGL |
| ATOM | 2464 | CG | PRO | 329 | 34.685 | 8.128 | 49.959 | 1.00 | 31.43 | BLGL |
| ATOM | 2465 | C | PRO | 329 | 33.966 | 4.520 | 49.614 | 1.00 | 29.93 | BLGL |
| ATOM | 2466 | O | PRO | 329 | 33.416 | 4.132 | 50.639 | 1.00 | 30.03 | BLGL |
| ATOM | 2467 | N | ALA | 330 | 34.582 | 3.706 | 48.768 | 1.00 | 29.86 | BLGL |
| ATOM | 2468 | CA | ALA | 330 | 34.614 | 2.272 | 48.987 | 1.00 | 32.93 | BLGL |
| ATOM | 2469 | CB | ALA | 330 | 35.343 | 1.585 | 47.833 | 1.00 | 31.50 | BLGL |
| ATOM | 2470 | C | ALA | 330 | 35.265 | 1.911 | 50.313 | 1.00 | 35.35 | BLGL |
| ATOM | 2471 | O | ALA | 330 | 34.894 | 0.916 | 50.940 | 1.00 | 35.56 | BLGL |
| ATOM | 2472 | N | HIS | 331 | 36.228 | 2.721 | 50.749 | 1.00 | 37.94 | BLGL |
| ATOM | 2473 | CA | HIS | 331 | 36.922 | 2.440 | 52.001 | 1.00 | 40.82 | BLGL |
| ATOM | 2474 | CB | HIS | 331 | 38.282 | 3.143 | 52.049 | 1.00 | 41.19 | BLGL |
| ATOM | 2475 | CG | HIS | 331 | 38.195 | 4.632 | 52.171 | 1.00 | 42.83 | BLGL |
| ATOM | 2476 | CD2 | HIS | 331 | 38.170 | 5.436 | 53.261 | 1.00 | 42.69 | BLGL |
| ATOM | 2477 | ND1 | HIS | 331 | 38.130 | 5.469 | 51.077 | 1.00 | 43.41 | BLGL |
| ATOM | 2478 | CE1 | HIS | 331 | 38.073 | 6.725 | 51.488 | 1.00 | 42.26 | BLGL |
| ATOM | 2479 | NE2 | HIS | 331 | 38.096 | 6.732 | 52.809 | 1.00 | 42.43 | BLGL |
| ATOM | 2480 | C | HIS | 331 | 36.130 | 2.805 | 53.254 | 1.00 | 42.32 | BLGL |
| ATOM | 2481 | O | HIS | 331 | 36.674 | 2.788 | 54.354 | 1.00 | 43.73 | BLGL |
| ATOM | 2482 | N | ARG | 332 | 34.857 | 3.149 | 53.105 | 1.00 | 43.54 | BLGL |
| ATOM | 2483 | CA | ARG | 332 | 34.041 | 3.478 | 54.264 | 1.00 | 43.67 | BLGL |
| ATOM | 2484 | CB | ARG | 332 | 33.446 | 4.878 | 54.152 | 1.00 | 46.16 | BLGL |
| ATOM | 2485 | CG | ARG | 332 | 34.428 | 6.031 | 54.232 | 1.00 | 51.93 | BLGL |
| ATOM | 2486 | CD | ARG | 332 | 33.693 | 7.258 | 54.754 | 1.00 | 55.92 | BLGL |
| ATOM | 2487 | NE | ARG | 332 | 32.323 | 7.299 | 54.240 | 1.00 | 62.04 | BLGL |
| ATOM | 2488 | CZ | ARG | 332 | 31.376 | 8.138 | 54.664 | 1.00 | 64.85 | BLGL |
| ATOM | 2489 | NH1 | ARG | 332 | 30.154 | 8.095 | 54.132 | 1.00 | 64.81 | BLGL |
| ATOM | 2490 | NH2 | ARG | 332 | 31.640 | 9.023 | 55.622 | 1.00 | 65.83 | BLGL |
| ATOM | 2491 | C | ARG | 332 | 32.899 | 2.482 | 54.368 | 1.00 | 43.46 | BLGL |
| ATOM | 2492 | O | ARG | 332 | 31.882 | 2.766 | 54.999 | 1.00 | 42.10 | BLGL |
| ATOM | 2493 | N | LEU | 333 | 33.077 | 1.318 | 53.748 | 1.00 | 43.54 | BLGL |
| ATOM | 2494 | CA | LEU | 333 | 32.058 | 0.277 | 53.739 | 1.00 | 44.90 | BLGL |
| ATOM | 2495 | CB | LEU | 333 | 32.700 | -1.104 | 53.605 | 1.00 | 44.71 | BLGL |
| ATOM | 2496 | CG | LEU | 333 | 32.076 | -1.981 | 52.511 | 1.00 | 47.14 | BLGL |
| ATOM | 2497 | CD1 | LEU | 333 | 32.702 | -3.370 | 52.561 | 1.00 | 47.53 | BLGL |
| ATOM | 2498 | CD2 | LEU | 333 | 30.561 | -2.068 | 52.691 | 1.00 | 46.62 | BLGL |
| ATOM | 2499 | C | LEU | 333 | 31.154 | 0.282 | 54.959 | 1.00 | 46.15 | BLGL |
| ATOM | 2500 | O | LEU | 333 | 29.931 | 0.378 | 54.833 | 1.00 | 47.20 | BLGL |
| ATOM | 2501 | N | GLU | 334 | 31.755 | 0.183 | 56.139 | 1.00 | 47.86 | BLGL |
| ATOM | 2502 | CA | GLU | 334 | 30.989 | 0.159 | 57.384 | 1.00 | 48.83 | BLGL |
| ATOM | 2503 | CB | GLU | 334 | 31.934 | 0.012 | 58.584 | 1.00 | 51.92 | BLGL |
| ATOM | 2504 | CG | GLU | 334 | 32.639 | -1.345 | 58.641 | 1.00 | 58.71 | BLGL |
| ATOM | 2505 | CD | GLU | 334 | 31.663 | -2.521 | 58.588 | 1.00 | 61.85 | BLGL |
| ATOM | 2506 | OE1 | GLU | 334 | 30.824 | -2.642 | 59.510 | 1.00 | 62.23 | BLGL |
| ATOM | 2507 | OE2 | GLU | 334 | 31.734 | -3.319 | 57.622 | 1.00 | 63.86 | BLGL |

# Fig. 4 cont.

| ATOM | 2508 | C    | GLU | 334 | 30.083 | 1.374  | 57.584 | 1.00 | 46.21 | BLGL |
|------|------|------|-----|-----|--------|--------|--------|------|-------|------|
| ATOM | 2509 | O    | GLU | 334 | 28.939 | 1.246  | 58.030 | 1.00 | 45.37 | BLGL |
| ATOM | 2510 | N    | LYS | 335 | 30.583 | 2.552  | 57.251 | 1.00 | 44.31 | BLGL |
| ATOM | 2511 | CA   | LYS | 335 | 29.783 | 3.752  | 57.415 | 1.00 | 43.94 | BLGL |
| ATOM | 2512 | CB   | LYS | 335 | 30.687 | 4.980  | 57.370 | 1.00 | 48.35 | BLGL |
| ATOM | 2513 | CG   | LYS | 335 | 30.158 | 6.168  | 58.168 | 1.00 | 51.85 | BLGL |
| ATOM | 2514 | CD   | LYS | 335 | 29.958 | 5.809  | 59.653 | 1.00 | 56.01 | BLGL |
| ATOM | 2515 | CE   | LYS | 335 | 31.207 | 5.161  | 60.270 | 1.00 | 57.13 | BLGL |
| ATOM | 2516 | NZ   | LYS | 335 | 32.440 | 5.982  | 60.078 | 1.00 | 58.45 | BLGL |
| ATOM | 2517 | C    | LYS | 335 | 28.717 | 3.843  | 56.318 | 1.00 | 42.75 | BLGL |
| ATOM | 2518 | O    | LYS | 335 | 27.664 | 4.458  | 56.508 | 1.00 | 40.92 | BLGL |
| ATOM | 2519 | N    | ASN | 336 | 28.999 | 3.229  | 55.169 | 1.00 | 40.89 | BLGL |
| ATOM | 2520 | CA   | ASN | 336 | 28.068 | 3.233  | 54.050 | 1.00 | 36.25 | BLGL |
| ATOM | 2521 | CB   | ASN | 336 | 28.758 | 2.764  | 52.774 | 1.00 | 34.22 | BLGL |
| ATOM | 2522 | CG   | ASN | 336 | 29.754 | 3.770  | 52.252 | 1.00 | 33.73 | BLGL |
| ATOM | 2523 | OD1  | ASN | 336 | 29.698 | 4.949  | 52.593 | 1.00 | 33.95 | BLGL |
| ATOM | 2524 | ND2  | ASN | 336 | 30.661 | 3.316  | 51.401 | 1.00 | 34.13 | BLGL |
| ATOM | 2525 | C    | ASN | 336 | 26.883 | 2.332  | 54.333 | 1.00 | 35.83 | BLGL |
| ATOM | 2526 | O    | ASN | 336 | 25.742 | 2.702  | 54.050 | 1.00 | 35.07 | BLGL |
| ATOM | 2527 | N    | LYS | 337 | 27.161 | 1.147  | 54.882 | 1.00 | 34.86 | BLGL |
| ATOM | 2528 | CA   | LYS | 337 | 26.116 | 0.171  | 55.209 | 1.00 | 33.18 | BLGL |
| ATOM | 2529 | CB   | LYS | 337 | 26.712 | -1.023 | 55.953 | 1.00 | 31.58 | BLGL |
| ATOM | 2530 | CG   | LYS | 337 | 27.594 | -1.901 | 55.095 | 1.00 | 32.46 | BLGL |
| ATOM | 2531 | CD   | LYS | 337 | 28.112 | -3.095 | 55.881 | 1.00 | 33.49 | BLGL |
| ATOM | 2532 | CE   | LYS | 337 | 28.869 | -4.046 | 54.967 | 1.00 | 38.20 | BLGL |
| ATOM | 2533 | NZ   | LYS | 337 | 29.366 | -5.262 | 55.679 | 1.00 | 41.08 | BLGL |
| ATOM | 2534 | C    | LYS | 337 | 25.042 | 0.812  | 56.069 | 1.00 | 32.37 | BLGL |
| ATOM | 2535 | O    | LYS | 337 | 23.866 | 0.477  | 55.971 | 1.00 | 30.10 | BLGL |
| ATOM | 2536 | N    | ALA | 338 | 25.466 | 1.738  | 56.917 | 1.00 | 32.27 | BLGL |
| ATOM | 2537 | CA   | ALA | 338 | 24.543 | 2.434  | 57.793 | 1.00 | 32.10 | BLGL |
| ATOM | 2538 | CB   | ALA | 338 | 25.313 | 3.383  | 58.712 | 1.00 | 30.46 | BLGL |
| ATOM | 2539 | C    | ALA | 338 | 23.533 | 3.211  | 56.951 | 1.00 | 31.53 | BLGL |
| ATOM | 2540 | O    | ALA | 338 | 22.332 | 3.174  | 57.217 | 1.00 | 32.87 | BLGL |
| ATOM | 2541 | N    | LEU | 339 | 24.025 | 3.915  | 55.937 | 1.00 | 29.75 | BLGL |
| ATOM | 2542 | CA   | LEU | 339 | 23.165 | 4.703  | 55.064 | 1.00 | 28.75 | BLGL |
| ATOM | 2543 | CB   | LEU | 339 | 24.019 | 5.580  | 54.149 | 1.00 | 29.58 | BLGL |
| ATOM | 2544 | CG   | LEU | 339 | 24.839 | 6.671  | 54.842 | 1.00 | 29.29 | BLGL |
| ATOM | 2545 | CD1  | LEU | 339 | 25.763 | 7.358  | 53.858 | 1.00 | 30.28 | BLGL |
| ATOM | 2546 | CD2  | LEU | 339 | 23.889 | 7.674  | 55.457 | 1.00 | 30.12 | BLGL |
| ATOM | 2547 | C    | LEU | 339 | 22.246 | 3.824  | 54.217 | 1.00 | 28.58 | BLGL |
| ATOM | 2548 | O    | LEU | 339 | 21.035 | 4.049  | 54.154 | 1.00 | 28.13 | BLGL |
| ATOM | 2549 | N    | TRP | 340 | 22.828 | 2.828  | 53.557 | 1.00 | 27.39 | BLGL |
| ATOM | 2550 | CA   | TRP | 340 | 22.052 | 1.925  | 52.719 | 1.00 | 26.49 | BLGL |
| ATOM | 2551 | CB   | TRP | 340 | 22.900 | 0.746  | 52.236 | 1.00 | 23.72 | BLGL |
| ATOM | 2552 | CG   | TRP | 340 | 24.091 | 1.114  | 51.444 | 1.00 | 22.86 | BLGL |
| ATOM | 2553 | CD2  | TRP | 340 | 25.305 | 0.366  | 51.336 | 1.00 | 23.48 | BLGL |
| ATOM | 2554 | CE2  | TRP | 340 | 26.154 | 1.077  | 50.458 | 1.00 | 23.45 | BLGL |
| ATOM | 2555 | CE3  | TRP | 340 | 25.760 | -0.839 | 51.895 | 1.00 | 23.20 | BLGL |
| ATOM | 2556 | CD1  | TRP | 340 | 24.243 | 2.214  | 50.651 | 1.00 | 22.87 | BLGL |
| ATOM | 2557 | NE1  | TRP | 340 | 25.480 | 2.200  | 50.056 | 1.00 | 22.68 | BLGL |
| ATOM | 2558 | CZ2  | TRP | 340 | 27.437 | 0.626  | 50.123 | 1.00 | 23.93 | BLGL |
| ATOM | 2559 | CZ3  | TRP | 340 | 27.036 | -1.288 | 51.561 | 1.00 | 24.91 | BLGL |
| ATOM | 2560 | CH2  | TRP | 340 | 27.859 | -0.553 | 50.682 | 1.00 | 23.29 | BLGL |
| ATOM | 2561 | C    | TRP | 340 | 20.891 | 1.359  | 53.505 | 1.00 | 26.35 | BLGL |
| ATOM | 2562 | O    | TRP | 340 | 19.777 | 1.252  | 53.005 | 1.00 | 26.95 | BLGL |
| ATOM | 2563 | N    | GLU | 341 | 21.179 | 0.990  | 54.743 | 1.00 | 27.03 | BLGL |
| ATOM | 2564 | CA   | GLU | 341 | 20.206 | 0.383  | 55.629 | 1.00 | 27.61 | BLGL |
| ATOM | 2565 | CB   | GLU | 341 | 20.939 | -0.239 | 56.818 | 1.00 | 29.81 | BLGL |
| ATOM | 2566 | CG   | GLU | 341 | 20.338 | -1.534 | 57.345 | 1.00 | 32.17 | BLGL |
| ATOM | 2567 | CD   | GLU | 341 | 20.490 | -2.693 | 56.384 | 1.00 | 34.50 | BLGL |
| ATOM | 2568 | OE1  | GLU | 341 | 20.087 | -3.811 | 56.756 | 1.00 | 38.21 | BLGL |
| ATOM | 2569 | OE2  | GLU | 341 | 21.003 | -2.503 | 55.261 | 1.00 | 35.23 | BLGL |
| ATOM | 2570 | C    | GLU | 341 | 19.150 | 1.366  | 56.112 | 1.00 | 27.16 | BLGL |
| ATOM | 2571 | O    | GLU | 341 | 17.967 | 1.044  | 56.169 | 1.00 | 27.02 | BLGL |
| ATOM | 2572 | N    | THR | 342 | 19.569 | 2.572  | 56.452 | 1.00 | 27.11 | BLGL |
| ATOM | 2573 | CA   | THR | 342 | 18.624 | 3.562  | 56.940 | 1.00 | 27.99 | BLGL |

# Fig. 4 cont.

| ATOM | 2574 | CB | THR | 342 | 19.356 | 4.706 | 57.658 | 1.00 | 27.99 | BLGL |
|------|------|------|-----|-----|--------|-------|--------|------|-------|------|
| ATOM | 2575 | OG1 | THR | 342 | 20.097 | 4.174 | 58.759 | 1.00 | 29.52 | BLGL |
| ATOM | 2576 | CG2 | THR | 342 | 18.365 | 5.731 | 58.173 | 1.00 | 28.27 | BLGL |
| ATOM | 2577 | C | THR | 342 | 17.732 | 4.169 | 55.860 | 1.00 | 27.72 | BLGL |
| ATOM | 2578 | O | THR | 342 | 16.527 | 4.283 | 56.047 | 1.00 | 27.61 | BLGL |
| ATOM | 2579 | N | TYR | 343 | 18.319 | 4.554 | 54.732 | 1.00 | 28.64 | BLGL |
| ATOM | 2580 | CA | TYR | 343 | 17.544 | 5.185 | 53.675 | 1.00 | 29.90 | BLGL |
| ATOM | 2581 | CB | TYR | 343 | 18.260 | 6.448 | 53.209 | 1.00 | 31.83 | BLGL |
| ATOM | 2582 | CG | TYR | 343 | 18.573 | 7.381 | 54.350 | 1.00 | 35.78 | BLGL |
| ATOM | 2583 | CD1 | TYR | 343 | 19.798 | 7.313 | 55.013 | 1.00 | 36.95 | BLGL |
| ATOM | 2584 | CE1 | TYR | 343 | 20.078 | 8.151 | 56.085 | 1.00 | 38.42 | BLGL |
| ATOM | 2585 | CD2 | TYR | 343 | 17.631 | 8.313 | 54.792 | 1.00 | 35.14 | BLGL |
| ATOM | 2586 | CE2 | TYR | 343 | 17.901 | 9.153 | 55.864 | 1.00 | 36.75 | BLGL |
| ATOM | 2587 | CZ | TYR | 343 | 19.128 | 9.067 | 56.503 | 1.00 | 38.36 | BLGL |
| ATOM | 2588 | OH | TYR | 343 | 19.417 | 9.904 | 57.554 | 1.00 | 40.88 | BLGL |
| ATOM | 2589 | C | TYR | 343 | 17.202 | 4.327 | 52.469 | 1.00 | 28.69 | BLGL |
| ATOM | 2590 | O | TYR | 343 | 16.524 | 4.788 | 51.554 | 1.00 | 28.30 | BLGL |
| ATOM | 2591 | N | GLY | 344 | 17.652 | 3.081 | 52.470 | 1.00 | 28.37 | BLGL |
| ATOM | 2592 | CA | GLY | 344 | 17.375 | 2.204 | 51.347 | 1.00 | 29.03 | BLGL |
| ATOM | 2593 | C | GLY | 344 | 18.001 | 2.730 | 50.068 | 1.00 | 28.56 | BLGL |
| ATOM | 2594 | O | GLY | 344 | 17.425 | 2.603 | 48.987 | 1.00 | 27.04 | BLGL |
| ATOM | 2595 | N | SER | 345 | 19.187 | 3.320 | 50.199 | 1.00 | 27.20 | BLGL |
| ATOM | 2596 | CA | SER | 345 | 19.903 | 3.888 | 49.067 | 1.00 | 25.65 | BLGL |
| ATOM | 2597 | CB | SER | 345 | 20.754 | 5.061 | 49.530 | 1.00 | 25.43 | BLGL |
| ATOM | 2598 | OG | SER | 345 | 21.600 | 4.654 | 50.582 | 1.00 | 31.71 | BLGL |
| ATOM | 2599 | C | SER | 345 | 20.780 | 2.853 | 48.380 | 1.00 | 25.28 | BLGL |
| ATOM | 2600 | O | SER | 345 | 21.554 | 3.183 | 47.479 | 1.00 | 24.47 | BLGL |
| ATOM | 2601 | N | GLY | 346 | 20.662 | 1.604 | 48.823 | 1.00 | 24.37 | BLGL |
| ATOM | 2602 | CA | GLY | 346 | 21.414 | 0.518 | 48.220 | 1.00 | 21.46 | BLGL |
| ATOM | 2603 | C | GLY | 346 | 20.430 | -0.252 | 47.360 | 1.00 | 20.92 | BLGL |
| ATOM | 2604 | O | GLY | 346 | 19.286 | 0.183 | 47.216 | 1.00 | 21.35 | BLGL |
| ATOM | 2605 | N | TRP | 347 | 20.834 | -1.385 | 46.795 | 1.00 | 18.57 | BLGL |
| ATOM | 2606 | CA | TRP | 347 | 19.915 | -2.145 | 45.959 | 1.00 | 18.47 | BLGL |
| ATOM | 2607 | CB | TRP | 347 | 20.677 | -3.115 | 45.057 | 1.00 | 19.55 | BLGL |
| ATOM | 2608 | CG | TRP | 347 | 20.976 | -4.426 | 45.700 | 1.00 | 24.39 | BLGL |
| ATOM | 2609 | CD2 | TRP | 347 | 20.205 | -5.626 | 45.576 | 1.00 | 26.03 | · BLGL |
| ATOM | 2610 | CE2 | TRP | 347 | 20.843 | -6.616 | 46.361 | 1.00 | 27.34 | BLGL |
| ATOM | 2611 | CE3 | TRP | 347 | 19.035 | -5.963 | 44.878 | 1.00 | 25.88 | BLGL |
| ATOM | 2612 | CD1 | TRP | 347 | 22.023 | -4.725 | 46.533 | 1.00 | 24.43 | BLGL |
| ATOM | 2613 | NE1 | TRP | 347 | 21.950 | -6.039 | 46.931 | 1.00 | 24.87 | BLGL |
| ATOM | 2614 | CZ2 | TRP | 347 | 20.344 | -7.926 | 46.467 | 1.00 | 27.61 | BLGL |
| ATOM | 2615 | CZ3 | TRP | 347 | 18.541 | -7.268 | 44.982 | 1.00 | 26.42 | BLGL |
| ATOM | 2616 | CH2 | TRP | 347 | 19.195 | -8.229 | 45.770 | 1.00 | 25.85 | BLGL |
| ATOM | 2617 | C | TRP | 347 | 18.910 | -2.916 | 46.807 | 1.00 | 17.94 | BLGL |
| ATOM | 2618 | O | TRP | 347 | 17.820 | -3.255 | 46.347 | 1.00 | 16.07 | BLGL |
| ATOM | 2619 | N | ALA | 348 | 19.296 | -3.197 | 48.047 | 1.00 | 19.28 | BLGL |
| ATOM | 2620 | CA | ALA | 348 | 18.444 | -3.918 | 48.984 | 1.00 | 21.94 | BLGL |
| ATOM | 2621 | CB | ALA | 348 | 18.387 | -5.394 | 48.607 | 1.00 | 20.51 | BLGL |
| ATOM | 2622 | C | ALA | 348 | 18.948 | -3.767 | 50.422 | 1.00 | 24.22 | BLGL |
| ATOM | 2623 | O | ALA | 348 | 20.138 | -3.549 | 50.659 | 1.00 | 25.24 | BLGL |
| ATOM | 2624 | N | THR | 349 | 18.030 | -3.870 | 51.379 | 1.00 | 25.44 | BLGL |
| ATOM | 2625 | CA | THR | 349 | 18.378 | -3.774 | 52.789 | 1.00 | 25.50 | BLGL |
| ATOM | 2626 | CB | THR | 349 | 17.509 | -2.738 | 53.553 | 1.00 | 26.44 | BLGL |
| ATOM | 2627 | OG1 | THR | 349 | 16.167 | -3.228 | 53.679 | 1.00 | 25.28 | BLGL |
| ATOM | 2628 | CG2 | THR | 349 | 17.500 | -1.400 | 52.823 | 1.00 | 24.16 | BLGL |
| ATOM | 2629 | C | THR | 349 | 18.102 | -5.139 | 53.383 | 1.00 | 26.30 | BLGL |
| ATOM | 2630 | O | THR | 349 | 17.382 | -5.942 | 52.791 | 1.00 | 26.26 | BLGL |
| ATOM | 2631 | N | SER | 350 | 18.671 | -5.403 | 54.551 | 1.00 | 27.06 | BLGL |
| ATOM | 2632 | CA | SER | 350 | 18.463 | -6.685 | 55.208 | 1.00 | 26.38 | BLGL |
| ATOM | 2633 | CB | SER | 350 | 19.252 | -6.738 | 56.514 | 1.00 | 23.71 | BLGL |
| ATOM | 2634 | OG | SER | 350 | 18.812 | -5.726 | 57.400 | 1.00 | 21.01 | BLGL |
| ATOM | 2635 | C | SER | 350 | 16.975 | -6.911 | 55.490 | 1.00 | 26.83 | BLGL |
| ATOM | 2636 | O | SER | 350 | 16.509 | -8.046 | 55.520 | 1.00 | 26.17 | BLGL |
| ATOM | 2637 | N | TYR | 351 | 16.225 | -5.830 | 55.683 | 1.00 | 28.04 | BLGL |
| ATOM | 2638 | CA | TYR | 351 | 14.796 | -5.946 | 55.965 | 1.00 | 30.41 | BLGL |
| ATOM | 2639 | CB | TYR | 351 | 14.208 | -4.566 | 56.244 | 1.00 | 32.17 | BLGL |

# Fig. 4 cont.

| ATOM | 2640 | CG | TYR | 351 | 14.911 | -3.829 | 57.352 | 1.00 | 33.63 | BLGL |
|------|------|-----|-----|-----|--------|--------|--------|------|-------|------|
| ATOM | 2641 | CD1 | TYR | 351 | 15.961 | -2.951 | 57.083 | 1.00 | 35.43 | BLGL |
| ATOM | 2642 | CE1 | TYR | 351 | 16.623 | -2.279 | 58.114 | 1.00 | 35.75 | BLGL |
| ATOM | 2643 | CD2 | TYR | 351 | 14.539 | -4.020 | 58.677 | 1.00 | 35.69 | BLGL |
| ATOM | 2644 | CE2 | TYR | 351 | 15.193 | -3.355 | 59.717 | 1.00 | 36.21 | BLGL |
| ATOM | 2645 | CZ | TYR | 351 | 16.231 | -2.488 | 59.427 | 1.00 | 35.60 | BLGL |
| ATOM | 2646 | OH | TYR | 351 | 16.865 | -1.828 | 60.451 | 1.00 | 36.59 | BLGL |
| ATOM | 2647 | C | TYR | 351 | 14.012 | -6.626 | 54.836 | 1.00 | 30.90 | BLGL |
| ATOM | 2648 | O | TYR | 351 | 12.921 | -7.159 | 55.055 | 1.00 | 30.86 | BLGL |
| ATOM | 2649 | N | ALA | 352 | 14.572 | -6.604 | 53.633 | 1.00 | 30.77 | BLGL |
| ATOM | 2650 | CA | ALA | 352 | 13.936 | -7.220 | 52.476 | 1.00 | 31.75 | BLGL |
| ATOM | 2651 | CB | ALA | 352 | 14.611 | -6.744 | 51.202 | 1.00 | 30.75 | BLGL |
| ATOM | 2652 | C | ALA | 352 | 13.989 | -8.745 | 52.545 | 1.00 | 33.29 | BLGL |
| ATOM | 2653 | O | ALA | 352 | 13.411 | -9.434 | 51.700 | 1.00 | 33.71 | BLGL |
| ATOM | 2654 | N | ALA | 353 | 14.680 | -9.273 | 53.549 | 1.00 | 33.30 | BLGL |
| ATOM | 2655 | CA | ALA | 353 | 14.804 | -10.718 | 53.706 | 1.00 | 33.02 | BLGL |
| ATOM | 2656 | CB | ALA | 353 | 15.687 | -11.033 | 54.908 | 1.00 | 34.24 | BLGL |
| ATOM | 2657 | C | ALA | 353 | 13.449 | -11.409 | 53.856 | 1.00 | 32.34 | BLGL |
| ATOM | 2658 | O | ALA | 353 | 13.270 | -12.545 | 53.422 | 1.00 | 30.15 | BLGL |
| ATOM | 2659 | N | GLU | 354 | 12.496 | -10.716 | 54.466 | 1.00 | 33.65 | BLGL |
| ATOM | 2660 | CA | GLU | 354 | 11.176 | -11.284 | 54.668 | 1.00 | 35.34 | BLGL |
| ATOM | 2661 | CB | GLU | 354 | 10.345 | -10.375 | 55.578 | 1.00 | 35.98 | BLGL |
| ATOM | 2662 | CG | GLU | 354 | 9.744 | -9.163 | 54.894 | 1.00 | 37.66 | BLGL |
| ATOM | 2663 | CD | GLU | 354 | 8.831 | -8.378 | 55.818 | 1.00 | 40.92 | BLGL |
| ATOM | 2664 | OE1 | GLU | 354 | 8.010 | -7.584 | 55.310 | 1.00 | 42.14 | BLGL |
| ATOM | 2665 | OE2 | GLU | 354 | 8.935 | -8.548 | 57.055 | 1.00 | 41.70 | BLGL |
| ATOM | 2666 | C | GLU | 354 | 10.437 | -11.503 | 53.343 | 1.00 | 36.54 | BLGL |
| ATOM | 2667 | O | GLU | 354 | 9.614 | -12.416 | 53.228 | 1.00 | 36.40 | BLGL |
| ATOM | 2668 | N | TYR | 355 | 10.735 | -10.673 | 52.345 | 1.00 | 36.32 | BLGL |
| ATOM | 2669 | CA | TYR | 355 | 10.072 | -10.778 | 51.046 | 1.00 | 35.27 | BLGL |
| ATOM | 2670 | CB | TYR | 355 | 9.800 | -9.381 | 50.496 | 1.00 | 32.38 | BLGL |
| ATOM | 2671 | CG | TYR | 355 | 8.715 | -9.339 | 49.445 | 1.00 | 32.93 | BLGL |
| ATOM | 2672 | CD1 | TYR | 355 | 9.022 | -9.211 | 48.087 | 1.00 | 31.94 | BLGL |
| ATOM | 2673 | CE1 | TYR | 355 | 8.014 | -9.141 | 47.126 | 1.00 | 30.60 | BLGL |
| ATOM | 2674 | CD2 | TYR | 355 | 7.372 | -9.403 | 49.812 | 1.00 | 31.34 | BLGL |
| ATOM | 2675 | CE2 | TYR | 355 | 6.364 | -9.333 | 48.864 | 1.00 | 31.48 | BLGL |
| ATOM | 2676 | CZ | TYR | 355 | 6.688 | -9.198 | 47.524 | 1.00 | 32.10 | BLGL |
| ATOM | 2677 | OH | TYR | 355 | 5.679 | -9.084 | 46.593 | 1.00 | 32.53 | BLGL |
| ATOM | 2678 | C | TYR | 355 | 10.873 | -11.590 | 50.034 | 1.00 | 36.46 | BLGL |
| ATOM | 2679 | O | TYR | 355 | 10.306 | -12.262 | 49.177 | 1.00 | 33.16 | BLGL |
| ATOM | 2680 | N | ASP | 356 | 12.196 | -11.513 | 50.133 | 1.00 | 39.53 | BLGL |
| ATOM | 2681 | CA | ASP | 356 | 13.079 | -12.251 | 49.241 | 1.00 | 42.86 | BLGL |
| ATOM | 2682 | CB | ASP | 356 | 13.568 | -11.355 | 48.096 | 1.00 | 43.64 | BLGL |
| ATOM | 2683 | CG | ASP | 356 | 14.568 | -12.064 | 47.182 | 1.00 | 44.35 | BLGL |
| ATOM | 2684 | OD1 | ASP | 356 | 15.202 | -11.382 | 46.349 | 1.00 | 42.98 | BLGL |
| ATOM | 2685 | OD2 | ASP | 356 | 14.715 | -13.303 | 47.293 | 1.00 | 45.31 | BLGL |
| ATOM | 2686 | C | ASP | 356 | 14.278 | -12.741 | 50.045 | 1.00 | 45.45 | BLGL |
| ATOM | 2687 | O | ASP | 356 | 15.302 | -12.058 | 50.133 | 1.00 | 47.13 | BLGL |
| ATOM | 2688 | N | PRO | 357 | 14.165 | -13.931 | 50.650 | 1.00 | 46.19 | BLGL |
| ATOM | 2689 | CD | PRO | 357 | 12.983 | -14.810 | 50.688 | 1.00 | 45.78 | BLGL |
| ATOM | 2690 | CA | PRO | 357 | 15.260 | -14.493 | 51.447 | 1.00 | 46.80 | BLGL |
| ATOM | 2691 | CB | PRO | 357 | 14.578 | -15.627 | 52.196 | 1.00 | 46.98 | BLGL |
| ATOM | 2692 | CG | PRO | 357 | 13.567 | -16.109 | 51.196 | 1.00 | 46.25 | BLGL |
| ATOM | 2693 | C | PRO | 357 | 16.412 | -14.990 | 50.581 | 1.00 | 48.11 | BLGL |
| ATOM | 2694 | O | PRO | 357 | 17.562 | -15.006 | 51.007 | 1.00 | 48.32 | BLGL |
| ATOM | 2695 | N | GLU | 358 | 16.075 | -15.381 | 49.358 | 1.00 | 49.36 | BLGL |
| ATOM | 2696 | CA | GLU | 358 | 17.019 | -15.911 | 48.385 | 1.00 | 51.27 | BLGL |
| ATOM | 2697 | CB | GLU | 358 | 16.257 | -16.304 | 47.125 | 1.00 | 53.72 | BLGL |
| ATOM | 2698 | CG | GLU | 358 | 15.040 | -17.170 | 47.389 | 1.00 | 58.04 | BLGL |
| ATOM | 2699 | CD | GLU | 358 | 15.414 | -18.587 | 47.774 | 1.00 | 62.05 | BLGL |
| ATOM | 2700 | OE1 | GLU | 358 | 15.886 | -19.331 | 46.886 | 1.00 | 63.62 | BLGL |
| ATOM | 2701 | OE2 | GLU | 358 | 15.244 | -18.955 | 48.961 | 1.00 | 64.62 | BLGL |
| ATOM | 2702 | C | GLU | 358 | 18.142 | -14.958 | 47.995 | 1.00 | 52.75 | BLGL |
| ATOM | 2703 | O | GLU | 358 | 19.319 | -15.232 | 48.240 | 1.00 | 53.92 | BLGL |
| ATOM | 2704 | N | ASP | 359 | 17.768 | -13.850 | 47.366 | 1.00 | 53.56 | BLGL |
| ATOM | 2705 | CA | ASP | 359 | 18.717 | -12.847 | 46.902 | 1.00 | 53.46 | BLGL |

# Fig. 4 cont.

| ATOM | 2706 | CB | ASP | 359 | 18.203 | -12.213 | 45.609 | 1.00 | 56.56 | BLGL |
|------|------|-----|-----|-----|--------|---------|--------|------|-------|------|
| ATOM | 2707 | CG | ASP | 359 | 18.748 | -12.887 | 44.366 | 1.00 | 58.60 | BLGL |
| ATOM | 2708 | OD1 | ASP | 359 | 18.654 | -14.130 | 44.268 | 1.00 | 60.63 | BLGL |
| ATOM | 2709 | OD2 | ASP | 359 | 19.268 | -12.166 | 43.485 | 1.00 | 59.51 | BLGL |
| ATOM | 2710 | C | ASP | 359 | 18.959 | -11.751 | 47.928 | 1.00 | 51.60 | BLGL |
| ATOM | 2711 | O | ASP | 359 | 19.876 | -11.837 | 48.742 | 1.00 | 50.90 | BLGL |
| ATOM | 2712 | N | ALA | 360 | 18.132 | -10.713 | 47.865 | 1.00 | 51.06 | BLGL |
| ATOM | 2713 | CA | ALA | 360 | 18.226 | -9.578 | 48.768 | 1.00 | 50.62 | BLGL |
| ATOM | 2714 | CB | ALA | 360 | 16.945 | -8.767 | 48.697 | 1.00 | 49.16 | BLGL |
| ATOM | 2715 | C | ALA | 360 | 18.471 | -10.058 | 50.193 | 1.00 | 50.90 | BLGL |
| ATOM | 2716 | O | ALA | 360 | 19.164 | -9.403 | 50.973 | 1.00 | 49.67 | BLGL |
| ATOM | 2717 | N | GLY | 361 | 17.896 | -11.214 | 50.515 | 1.00 | 52.39 | BLGL |
| ATOM | 2718 | CA | GLY | 361 | 18.042 | -11.794 | 51.837 | 1.00 | 52.85 | BLGL |
| ATOM | 2719 | C | GLY | 361 | 19.481 | -11.858 | 52.312 | 1.00 | 53.39 | BLGL |
| ATOM | 2720 | O | GLY | 361 | 19.809 | -11.331 | 53.378 | 1.00 | 54.42 | BLGL |
| ATOM | 2721 | N | LYS | 362 | 20.351 | -12.496 | 51.540 | 1.00 | 53.32 | BLGL |
| ATOM | 2722 | CA | LYS | 362 | 21.737 | -12.588 | 51.954 | 1.00 | 54.47 | BLGL |
| ATOM | 2723 | CB | LYS | 362 | 22.081 | -14.037 | 52.329 | 1.00 | 57.86 | BLGL |
| ATOM | 2724 | CG | LYS | 362 | 21.401 | -15.120 | 51.495 | 1.00 | 59.76 | BLGL |
| ATOM | 2725 | CD | LYS | 362 | 22.199 | -15.482 | 50.251 | 1.00 | 61.95 | BLGL |
| ATOM | 2726 | CE | LYS | 362 | 21.745 | -16.833 | 49.698 | 1.00 | 63.37 | BLGL |
| ATOM | 2727 | NZ | LYS | 362 | 22.557 | -17.264 | 48.522 | 1.00 | 62.07 | BLGL |
| ATOM | 2728 | C | LYS | 362 | 22.741 | -12.034 | 50.953 | 1.00 | 53.61 | BLGL |
| ATOM | 2729 | O | LYS | 362 | 23.823 | -12.595 | 50.770 | 1.00 | 54.78 | BLGL |
| ATOM | 2730 | N | TRP | 363 | 22.376 | -10.921 | 50.323 | 1.00 | 52.09 | BLGL |
| ATOM | 2731 | CA | TRP | 363 | 23.236 | -10.246 | 49.357 | 1.00 | 49.55 | BLGL |
| ATOM | 2732 | CB | TRP | 363 | 23.048 | -10.816 | 47.948 | 1.00 | 53.13 | BLGL |
| ATOM | 2733 | CG | TRP | 363 | 23.559 | -12.215 | 47.792 | 1.00 | 58.47 | BLGL |
| ATOM | 2734 | CD2 | TRP | 363 | 24.840 | -12.716 | 48.201 | 1.00 | 61.21 | BLGL |
| ATOM | 2735 | CE2 | TRP | 363 | 24.867 | -14.096 | 47.894 | 1.00 | 62.60 | BLGL |
| ATOM | 2736 | CE3 | TRP | 363 | 25.966 | -12.135 | 48.802 | 1.00 | 63.42 | BLGL |
| ATOM | 2737 | CD1 | TRP | 363 | 22.885 | -13.277 | 47.262 | 1.00 | 60.70 | BLGL |
| ATOM | 2738 | NE1 | TRP | 363 | 23.663 | -14.412 | 47.320 | 1.00 | 62.38 | BLGL |
| ATOM | 2739 | CZ2 | TRP | 363 | 25.981 | -14.907 | 48.168 | 1.00 | 63.65 | BLGL |
| ATOM | 2740 | CZ3 | TRP | 363 | 27.076 | -12.945 | 49.076 | 1.00 | 64.57 | BLGL |
| ATOM | 2741 | CH2 | TRP | 363 | 27.071 | -14.315 | 48.757 | 1.00 | 63.75 | BLGL |
| ATOM | 2742 | C | TRP | 363 | 22.900 | -8.765 | 49.354 | 1.00 | 45.74 | BLGL |
| ATOM | 2743 | O | TRP | 363 | 23.315 | -8.031 | 48.460 | 1.00 | 46.95 | BLGL |
| ATOM | 2744 | N | PHE | 364 | 22.143 | -8.333 | 50.357 | 1.00 | 40.08 | BLGL |
| ATOM | 2745 | CA | PHE | 364 | 21.748 | -6.939 | 50.478 | 1.00 | 36.02 | BLGL |
| ATOM | 2746 | CB | PHE | 364 | 20.798 | -6.763 | 51.664 | 1.00 | 35.97 | BLGL |
| ATOM | 2747 | CG | PHE | 364 | 21.393 | -7.163 | 52.989 | 1.00 | 35.49 | BLGL |
| ATOM | 2748 | CD1 | PHE | 364 | 22.170 | -6.264 | 53.723 | 1.00 | 34.51 | BLGL |
| ATOM | 2749 | CD2 | PHE | 364 | 21.194 | -8.448 | 53.493 | 1.00 | 34.67 | BLGL |
| ATOM | 2750 | CE1 | PHE | 364 | 22.739 | -6.637 | 54.937 | 1.00 | 33.03 | BLGL |
| ATOM | 2751 | CE2 | PHE | 364 | 21.759 | -8.834 | 54.705 | 1.00 | 33.39 | BLGL |
| ATOM | 2752 | CZ | PHE | 364 | 22.534 | -7.927 | 55.429 | 1.00 | 33.77 | BLGL |
| ATOM | 2753 | C | PHE | 364 | 22.978 | -6.061 | 50.655 | 1.00 | 33.99 | BLGL |
| ATOM | 2754 | O | PHE | 364 | 23.998 | -6.506 | 51.181 | 1.00 | 34.27 | BLGL |
| ATOM | 2755 | N | GLY | 365 | 22.881 | -4.816 | 50.208 | 1.00 | 30.67 | BLGL |
| ATOM | 2756 | CA | GLY | 365 | 24.008 | -3.915 | 50.322 | 1.00 | 28.90 | BLGL |
| ATOM | 2757 | C | GLY | 365 | 23.806 | -2.610 | 49.581 | 1.00 | 27.08 | BLGL |
| ATOM | 2758 | O | GLY | 365 | 22.708 | -2.058 | 49.571 | 1.00 | 27.26 | BLGL |
| ATOM | 2759 | N | GLY | 366 | 24.863 | -2.122 | 48.943 | 1.00 | 26.06 | BLGL |
| ATOM | 2760 | CA | GLY | 366 | 24.777 | -0.860 | 48.230 | 1.00 | 22.87 | BLGL |
| ATOM | 2761 | C | GLY | 366 | 24.434 | -0.934 | 46.757 | 1.00 | 22.45 | BLGL |
| ATOM | 2762 | O | GLY | 366 | 23.680 | -1.800 | 46.312 | 1.00 | 20.99 | BLGL |
| ATOM | 2763 | N | SER | 367 | 24.996 | 0.004 | 46.002 | 1.00 | 22.77 | BLGL |
| ATOM | 2764 | CA | SER | 367 | 24.779 | 0.098 | 44.566 | 1.00 | 21.36 | BLGL |
| ATOM | 2765 | CB | SER | 367 | 25.081 | 1.511 | 44.079 | 1.00 | 19.13 | BLGL |
| ATOM | 2766 | OG | SER | 367 | 25.081 | 1.539 | 42.665 | 1.00 | 20.78 | BLGL |
| ATOM | 2767 | C | SER | 367 | 25.649 | -0.877 | 43.802 | 1.00 | 20.92 | BLGL |
| ATOM | 2768 | O | SER | 367 | 26.828 | -1.040 | 44.111 | 1.00 | 22.00 | BLGL |
| ATOM | 2769 | N | ALA | 368 | 25.072 | -1.518 | 42.794 | 1.00 | 19.58 | BLGL |
| ATOM | 2770 | CA | ALA | 368 | 25.823 | -2.474 | 41.992 | 1.00 | 19.49 | BLGL |
| ATOM | 2771 | CB | ALA | 368 | 25.069 | -3.792 | 41.921 | 1.00 | 18.00 | BLGL |

# Fig. 4 cont.

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 2772 | C | ALA | 368 | 26.058 | −1.928 | 40.595 | 1.00 | 19.35 | BLGL |
| ATOM | 2773 | O | ALA | 368 | 26.610 | −2.612 | 39.735 | 1.00 | 19.98 | BLGL |
| ATOM | 2774 | N | VAL | 369 | 25.656 | −0.679 | 40.387 | 1.00 | 19.26 | BLGL |
| ATOM | 2775 | CA | VAL | 369 | 25.775 | −0.041 | 39.080 | 1.00 | 19.71 | BLGL |
| ATOM | 2776 | CB | VAL | 369 | 24.391 | 0.041 | 38.379 | 1.00 | 16.72 | BLGL |
| ATOM | 2777 | CG1 | VAL | 369 | 23.863 | −1.349 | 38.093 | 1.00 | 13.08 | BLGL |
| ATOM | 2778 | CG2 | VAL | 369 | 23.411 | 0.804 | 39.265 | 1.00 | 10.69 | BLGL |
| ATOM | 2779 | C | VAL | 369 | 26.357 | 1.366 | 39.124 | 1.00 | 20.80 | BLGL |
| ATOM | 2780 | O | VAL | 369 | 26.139 | 2.156 | 38.201 | 1.00 | 21.48 | BLGL |
| ATOM | 2781 | N | ASP | 370 | 27.083 | 1.693 | 40.187 | 1.00 | 21.01 | BLGL |
| ATOM | 2782 | CA | ASP | 370 | 27.680 | 3.024 | 40.269 | 1.00 | 21.96 | BLGL |
| ATOM | 2783 | CB | ASP | 370 | 28.401 | 3.226 | 41.617 | 1.00 | 20.78 | BLGL |
| ATOM | 2784 | CG | ASP | 370 | 29.224 | 2.016 | 42.042 | 1.00 | 26.31 | BLGL |
| ATOM | 2785 | OD1 | ASP | 370 | 28.640 | 1.027 | 42.529 | 1.00 | 27.68 | BLGL |
| ATOM | 2786 | OD2 | ASP | 370 | 30.466 | 2.045 | 41.893 | 1.00 | 31.81 | BLGL |
| ATOM | 2787 | C | ASP | 370 | 28.649 | 3.264 | 39.098 | 1.00 | 21.03 | BLGL |
| ATOM | 2788 | O | ASP | 370 | 28.886 | 4.405 | 38.695 | 1.00 | 16.48 | BLGL |
| ATOM | 2789 | N | ASN | 371 | 29.188 | 2.181 | 38.542 | 1.00 | 20.75 | BLGL |
| ATOM | 2790 | CA | ASN | 371 | 30.126 | 2.291 | 37.431 | 1.00 | 21.39 | BLGL |
| ATOM | 2791 | CB | ASN | 371 | 31.159 | 1.161 | 37.506 | 1.00 | 19.36 | BLGL |
| ATOM | 2792 | CG | ASN | 371 | 30.554 | −0.202 | 37.257 | 1.00 | 17.69 | BLGL |
| ATOM | 2793 | OD1 | ASN | 371 | 29.412 | −0.471 | 37.631 | 1.00 | 16.68 | BLGL |
| ATOM | 2794 | ND2 | ASN | 371 | 31.329 | −1.081 | 36.635 | 1.00 | 15.28 | BLGL |
| ATOM | 2795 | C | ASN | 371 | 29.435 | 2.298 | 36.062 | 1.00 | 22.85 | BLGL |
| ATOM | 2796 | O | ASN | 371 | 30.088 | 2.203 | 35.018 | 1.00 | 21.45 | BLGL |
| ATOM | 2797 | N | GLN | 372 | 28.109 | 2.405 | 36.074 | 1.00 | 21.57 | BLGL |
| ATOM | 2798 | CA | GLN | 372 | 27.355 | 2.458 | 34.837 | 1.00 | 21.91 | BLGL |
| ATOM | 2799 | CB | GLN | 372 | 26.432 | 1.248 | 34.702 | 1.00 | 19.34 | BLGL |
| ATOM | 2800 | CG | GLN | 372 | 27.186 | −0.043 | 34.541 | 1.00 | 19.05 | BLGL |
| ATOM | 2801 | CD | GLN | 372 | 26.332 | −1.154 | 33.981 | 1.00 | 18.53 | BLGL |
| ATOM | 2802 | OE1 | GLN | 372 | 25.802 | −1.043 | 32.881 | 1.00 | 16.76 | BLGL |
| ATOM | 2803 | NE2 | GLN | 372 | 26.199 | −2.240 | 34.732 | 1.00 | 19.99 | BLGL |
| ATOM | 2804 | C | GLN | 372 | 26.550 | 3.750 | 34.783 | 1.00 | 22.49 | BLGL |
| ATOM | 2805 | O | GLN | 372 | 25.693 | 3.927 | 33.920 | 1.00 | 24.48 | BLGL |
| ATOM | 2806 | N | ALA | 373 | 26.842 | 4.658 | 35.705 | 1.00 | 21.34 | BLGL |
| ATOM | 2807 | CA | ALA | 373 | 26.155 | 5.940 | 35.755 | 1.00 | 21.66 | BLGL |
| ATOM | 2808 | CB | ALA | 373 | 26.301 | 6.544 | 37.148 | 1.00 | 20.20 | BLGL |
| ATOM | 2809 | C | ALA | 373 | 26.702 | 6.914 | 34.705 | 1.00 | 22.35 | BLGL |
| ATOM | 2810 | O | ALA | 373 | 27.707 | 6.638 | 34.038 | 1.00 | 21.94 | BLGL |
| ATOM | 2811 | N | LEU | 374 | 26.025 | 8.048 | 34.555 | 1.00 | 21.60 | BLGL |
| ATOM | 2812 | CA | LEU | 374 | 26.454 | 9.080 | 33.617 | 1.00 | 21.79 | BLGL |
| ATOM | 2813 | CB | LEU | 374 | 25.273 | 9.548 | 32.763 | 1.00 | 19.88 | BLGL |
| ATOM | 2814 | CG | LEU | 374 | 24.631 | 8.408 | 31.962 | 1.00 | 19.67 | BLGL |
| ATOM | 2815 | CD1 | LEU | 374 | 23.430 | 8.928 | 31.196 | 1.00 | 19.92 | BLGL |
| ATOM | 2816 | CD2 | LEU | 374 | 25.650 | 7.809 | 31.011 | 1.00 | 17.34 | BLGL |
| ATOM | 2817 | C | LEU | 374 | 27.040 | 10.236 | 34.431 | 1.00 | 22.87 | BLGL |
| ATOM | 2818 | O | LEU | 374 | 27.314 | 11.319 | 33.905 | 1.00 | 21.82 | BLGL |
| ATOM | 2819 | N | PHE | 375 | 27.214 | 9.981 | 35.728 | 1.00 | 21.81 | BLGL |
| ATOM | 2820 | CA | PHE | 375 | 27.800 | 10.937 | 36.664 | 1.00 | 23.69 | BLGL |
| ATOM | 2821 | CB | PHE | 375 | 26.780 | 11.387 | 37.722 | 1.00 | 22.43 | BLGL |
| ATOM | 2822 | CG | PHE | 375 | 25.641 | 12.195 | 37.169 | 1.00 | 24.54 | BLGL |
| ATOM | 2823 | CD1 | PHE | 375 | 24.652 | 11.592 | 36.389 | 1.00 | 24.54 | BLGL |
| ATOM | 2824 | CD2 | PHE | 375 | 25.563 | 13.566 | 37.407 | 1.00 | 22.99 | BLGL |
| ATOM | 2825 | CE1 | PHE | 375 | 23.606 | 12.343 | 35.856 | 1.00 | 21.26 | BLGL |
| ATOM | 2826 | CE2 | PHE | 375 | 24.521 | 14.324 | 36.877 | 1.00 | 20.60 | BLGL |
| ATOM | 2827 | CZ | PHE | 375 | 23.543 | 13.712 | 36.101 | 1.00 | 22.10 | BLGL |
| ATOM | 2828 | C | PHE | 375 | 28.928 | 10.184 | 37.356 | 1.00 | 24.96 | BLGL |
| ATOM | 2829 | O | PHE | 375 | 28.849 | 8.963 | 37.505 | 1.00 | 26.41 | BLGL |
| ATOM | 2830 | N | ASP | 376 | 29.975 | 10.890 | 37.771 | 1.00 | 24.80 | BLGL |
| ATOM | 2831 | CA | ASP | 376 | 31.070 | 10.217 | 38.449 | 1.00 | 24.64 | BLGL |
| ATOM | 2832 | CB | ASP | 376 | 32.369 | 11.030 | 38.382 | 1.00 | 25.91 | BLGL |
| ATOM | 2833 | CG | ASP | 376 | 32.243 | 12.411 | 39.007 | 1.00 | 26.81 | BLGL |
| ATOM | 2834 | OD1 | ASP | 376 | 31.528 | 12.566 | 40.022 | 1.00 | 26.23 | BLGL |
| ATOM | 2835 | OD2 | ASP | 376 | 32.885 | 13.343 | 38.484 | 1.00 | 27.73 | BLGL |
| ATOM | 2836 | C | ASP | 376 | 30.698 | 9.969 | 39.899 | 1.00 | 24.00 | BLGL |
| ATOM | 2837 | O | ASP | 376 | 29.621 | 10.349 | 40.344 | 1.00 | 22.18 | BLGL |

# Fig. 4 cont.

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 2838 | N | PHE | 377 | 31.610 | 9.333 | 40.625 | 1.00 | 24.93 | BLGL |
| ATOM | 2839 | CA | PHE | 377 | 31.421 | 9.000 | 42.030 | 1.00 | 26.87 | BLGL |
| ATOM | 2840 | CB | PHE | 377 | 32.652 | 8.256 | 42.530 | 1.00 | 24.91 | BLGL |
| ATOM | 2841 | CG | PHE | 377 | 32.915 | 6.967 | 41.811 | 1.00 | 26.64 | BLGL |
| ATOM | 2842 | CD1 | PHE | 377 | 34.185 | 6.394 | 41.837 | 1.00 | 27.20 | BLGL |
| ATOM | 2843 | CD2 | PHE | 377 | 31.891 | 6.298 | 41.141 | 1.00 | 27.03 | BLGL |
| ATOM | 2844 | CE1 | PHE | 377 | 34.434 | 5.168 | 41.209 | 1.00 | 27.98 | BLGL |
| ATOM | 2845 | CE2 | PHE | 377 | 32.127 | 5.073 | 40.511 | 1.00 | 27.70 | BLGL |
| ATOM | 2846 | CZ | PHE | 377 | 33.402 | 4.505 | 40.546 | 1.00 | 28.28 | BLGL |
| ATOM | 2847 | C | PHE | 377 | 31.162 | 10.214 | 42.919 | 1.00 | 28.76 | BLGL |
| ATOM | 2848 | O | PHE | 377 | 30.660 | 10.084 | 44.041 | 1.00 | 29.47 | BLGL |
| ATOM | 2849 | N | LYS | 378 | 31.500 | 11.393 | 42.410 | 1.00 | 30.92 | BLGL |
| ATOM | 2850 | CA | LYS | 378 | 31.322 | 12.634 | 43.155 | 1.00 | 32.99 | BLGL |
| ATOM | 2851 | CB | LYS | 378 | 32.533 | 13.546 | 42.927 | 1.00 | 36.98 | BLGL |
| ATOM | 2852 | CG | LYS | 378 | 33.889 | 12.924 | 43.274 | 1.00 | 39.50 | BLGL |
| ATOM | 2853 | CD | LYS | 378 | 34.230 | 13.053 | 44.759 | 1.00 | 43.64 | BLGL |
| ATOM | 2854 | CE | LYS | 378 | 33.249 | 12.300 | 45.651 | 1.00 | 45.28 | BLGL |
| ATOM | 2855 | NZ | LYS | 378 | 33.467 | 12.607 | 47.092 | 1.00 | 46.72 | BLGL |
| ATOM | 2856 | C | LYS | 378 | 30.040 | 13.391 | 42.800 | 1.00 | 32.50 | BLGL |
| ATOM | 2857 | O | LYS | 378 | 29.803 | 14.487 | 43.309 | 1.00 | 31.66 | BLGL |
| ATOM | 2858 | N | GLY | 379 | 29.224 | 12.816 | 41.919 | 1.00 | 32.04 | BLGL |
| ATOM | 2859 | CA | GLY | 379 | 27.975 | 13.453 | 41.544 | 1.00 | 32.10 | BLGL |
| ATOM | 2860 | C | GLY | 379 | 28.092 | 14.430 | 40.397 | 1.00 | 33.14 | BLGL |
| ATOM | 2861 | O | GLY | 379 | 27.146 | 15.159 | 40.085 | 1.00 | 32.60 | BLGL |
| ATOM | 2862 | N | ARG | 380 | 29.261 | 14.451 | 39.771 | 1.00 | 35.05 | BLGL |
| ATOM | 2863 | CA | ARG | 380 | 29.507 | 15.342 | 38.647 | 1.00 | 35.69 | BLGL |
| ATOM | 2864 | CB | ARG | 380 | 30.958 | 15.817 | 38.660 | 1.00 | 40.31 | BLGL |
| ATOM | 2865 | CG | ARG | 380 | 31.123 | 17.323 | 38.592 | 1.00 | 48.35 | BLGL |
| ATOM | 2866 | CD | ARG | 380 | 32.569 | 17.728 | 38.876 | 1.00 | 55.04 | BLGL |
| ATOM | 2867 | NE | ARG | 380 | 33.058 | 17.213 | 40.164 | 1.00 | 61.15 | BLGL |
| ATOM | 2868 | CZ | ARG | 380 | 33.782 | 16.100 | 40.318 | 1.00 | 61.98 | BLGL |
| ATOM | 2869 | NH1 | ARG | 380 | 34.117 | 15.362 | 39.267 | 1.00 | 62.74 | BLGL |
| ATOM | 2870 | NH2 | ARG | 380 | 34.178 | 15.720 | 41.529 | 1.00 | 60.75 | BLGL |
| ATOM | 2871 | C | ARG | 380 | 29.216 | 14.587 | 37.354 | 1.00 | 34.09 | BLGL |
| ATOM | 2872 | O | ARG | 380 | 29.551 | 13.404 | 37.213 | 1.00 | 34.62 | BLGL |
| ATOM | 2873 | N | PRO | 381 | 28.590 | 15.265 | 36.386 | 1.00 | 30.20 | BLGL |
| ATOM | 2874 | CD | PRO | 381 | 28.201 | 16.683 | 36.407 | 1.00 | 27.18 | BLGL |
| ATOM | 2875 | CA | PRO | 381 | 28.250 | 14.653 | 35.101 | 1.00 | 28.29 | BLGL |
| ATOM | 2876 | CB | PRO | 381 | 27.395 | 15.723 | 34.438 | 1.00 | 27.26 | BLGL |
| ATOM | 2877 | CG | PRO | 381 | 28.018 | 16.980 | 34.941 | 1.00 | 26.31 | BLGL |
| ATOM | 2878 | C | PRO | 381 | 29.453 | 14.278 | 34.260 | 1.00 | 26.53 | BLGL |
| ATOM | 2879 | O | PRO | 381 | 30.436 | 15.014 | 34.221 | 1.00 | 27.34 | BLGL |
| ATOM | 2880 | N | LEU | 382 | 29.370 | 13.122 | 33.601 | 1.00 | 26.02 | BLGL |
| ATOM | 2881 | CA | LEU | 382 | 30.439 | 12.645 | 32.721 | 1.00 | 24.03 | BLGL |
| ATOM | 2882 | CB | LEU | 382 | 30.475 | 11.116 | 32.656 | 1.00 | 21.52 | BLGL |
| ATOM | 2883 | CG | LEU | 382 | 30.769 | 10.338 | 33.934 | 1.00 | 22.08 | BLGL |
| ATOM | 2884 | CD1 | LEU | 382 | 30.549 | 8.867 | 33.678 | 1.00 | 21.34 | BLGL |
| ATOM | 2885 | CD2 | LEU | 382 | 32.190 | 10.608 | 34.390 | 1.00 | 21.32 | BLGL |
| ATOM | 2886 | C | LEU | 382 | 30.128 | 13.174 | 31.336 | 1.00 | 23.10 | BLGL |
| ATOM | 2887 | O | LEU | 382 | 28.964 | 13.412 | 30.996 | 1.00 | 22.81 | BLGL |
| ATOM | 2888 | N | PRO | 383 | 31.160 | 13.364 | 30.511 | 1.00 | 22.83 | BLGL |
| ATOM | 2889 | CD | PRO | 383 | 32.593 | 13.134 | 30.744 | 1.00 | 21.59 | BLGL |
| ATOM | 2890 | CA | PRO | 383 | 30.919 | 13.873 | 29.159 | 1.00 | 22.58 | BLGL |
| ATOM | 2891 | CB | PRO | 383 | 32.327 | 13.950 | 28.559 | 1.00 | 22.02 | BLGL |
| ATOM | 2892 | CG | PRO | 383 | 33.101 | 12.953 | 29.345 | 1.00 | 23.42 | BLGL |
| ATOM | 2893 | C | PRO | 383 | 29.959 | 13.008 | 28.340 | 1.00 | 22.29 | BLGL |
| ATOM | 2894 | O | PRO | 383 | 29.346 | 13.491 | 27.395 | 1.00 | 23.29 | BLGL |
| ATOM | 2895 | N | SER | 384 | 29.815 | 11.739 | 28.718 | 1.00 | 23.07 | BLGL |
| ATOM | 2896 | CA | SER | 384 | 28.918 | 10.830 | 28.014 | 1.00 | 23.32 | BLGL |
| ATOM | 2897 | CB | SER | 384 | 29.189 | 9.387 | 28.438 | 1.00 | 23.43 | BLGL |
| ATOM | 2898 | OG | SER | 384 | 28.997 | 9.221 | 29.827 | 1.00 | 22.72 | BLGL |
| ATOM | 2899 | C | SER | 384 | 27.441 | 11.166 | 28.253 | 1.00 | 24.76 | BLGL |
| ATOM | 2900 | O | SER | 384 | 26.556 | 10.584 | 27.629 | 1.00 | 25.96 | BLGL |
| ATOM | 2901 | N | LEU | 385 | 27.166 | 12.094 | 29.160 | 1.00 | 23.88 | BLGL |
| ATOM | 2902 | CA | LEU | 385 | 25.792 | 12.474 | 29.419 | 1.00 | 24.72 | BLGL |
| ATOM | 2903 | CB | LEU | 385 | 25.721 | 13.380 | 30.644 | 1.00 | 22.46 | BLGL |

# Fig. 4 cont.

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 2904 | CG | LEU | 385 | 24.332 | 13.873 | 31.055 | 1.00 | 23.33 | BLGL |
| ATOM | 2905 | CD1 | LEU | 385 | 23.424 | 12.687 | 31.367 | 1.00 | 22.86 | BLGL |
| ATOM | 2906 | CD2 | LEU | 385 | 24.458 | 14.778 | 32.268 | 1.00 | 20.09 | BLGL |
| ATOM | 2907 | C | LEU | 385 | 25.250 | 13.207 | 28.193 | 1.00 | 26.26 | BLGL |
| ATOM | 2908 | O | LEU | 385 | 24.041 | 13.255 | 27.958 | 1.00 | 25.15 | BLGL |
| ATOM | 2909 | N | HIS | 386 | 26.161 | 13.763 | 27.404 | 1.00 | 28.46 | BLGL |
| ATOM | 2910 | CA | HIS | 386 | 25.789 | 14.512 | 26.213 | 1.00 | 32.60 | BLGL |
| ATOM | 2911 | CB | HIS | 386 | 26.937 | 15.437 | 25.816 | 1.00 | 37.77 | BLGL |
| ATOM | 2912 | CG | HIS | 386 | 27.172 | 16.539 | 26.799 | 1.00 | 45.65 | BLGL |
| ATOM | 2913 | CD2 | HIS | 386 | 26.393 | 17.016 | 27.801 | 1.00 | 45.94 | BLGL |
| ATOM | 2914 | ND1 | HIS | 386 | 28.330 | 17.291 | 26.820 | 1.00 | 48.26 | BLGL |
| ATOM | 2915 | CE1 | HIS | 386 | 28.254 | 18.180 | 27.795 | 1.00 | 49.16 | BLGL |
| ATOM | 2916 | NE2 | HIS | 386 | 27.089 | 18.033 | 28.405 | 1.00 | 49.07 | BLGL |
| ATOM | 2917 | C | HIS | 386 | 25.392 | 13.656 | 25.025 | 1.00 | 32.02 | BLGL |
| ATOM | 2918 | O | HIS | 386 | 25.011 | 14.184 | 23.979 | 1.00 | 34.90 | BLGL |
| ATOM | 2919 | N | VAL | 387 | 25.467 | 12.341 | 25.177 | 1.00 | 29.53 | BLGL |
| ATOM | 2920 | CA | VAL | 387 | 25.117 | 11.461 | 24.075 | 1.00 | 27.58 | BLGL |
| ATOM | 2921 | CB | VAL | 387 | 25.236 | 9.974 | 24.496 | 1.00 | 27.23 | BLGL |
| ATOM | 2922 | CG1 | VAL | 387 | 24.191 | 9.637 | 25.547 | 1.00 | 25.13 | BLGL |
| ATOM | 2923 | CG2 | VAL | 387 | 25.114 | 9.072 | 23.276 | 1.00 | 23.77 | BLGL |
| ATOM | 2924 | C | VAL | 387 | 23.701 | 11.760 | 23.572 | 1.00 | 26.94 | BLGL |
| ATOM | 2925 | O | VAL | 387 | 23.450 | 11.750 | 22.369 | 1.00 | 26.81 | BLGL |
| ATOM | 2926 | N | PHE | 388 | 22.788 | 12.060 | 24.491 | 1.00 | 25.61 | BLGL |
| ATOM | 2927 | CA | PHE | 388 | 21.403 | 12.339 | 24.136 | 1.00 | 26.79 | BLGL |
| ATOM | 2928 | CB | PHE | 388 | 20.586 | 12.619 | 25.390 | 1.00 | 25.81 | BLGL |
| ATOM | 2929 | CG | PHE | 388 | 20.433 | 11.432 | 26.272 | 1.00 | 26.19 | BLGL |
| ATOM | 2930 | CD1 | PHE | 388 | 21.003 | 11.412 | 27.536 | 1.00 | 27.32 | BLGL |
| ATOM | 2931 | CD2 | PHE | 388 | 19.728 | 10.317 | 25.834 | 1.00 | 25.78 | BLGL |
| ATOM | 2932 | CE1 | PHE | 388 | 20.873 | 10.300 | 28.355 | 1.00 | 27.00 | BLGL |
| ATOM | 2933 | CE2 | PHE | 388 | 19.592 | 9.198 | 26.647 | 1.00 | 26.04 | BLGL |
| ATOM | 2934 | CZ | PHE | 388 | 20.166 | 9.189 | 27.909 | 1.00 | 26.12 | BLGL |
| ATOM | 2935 | C | PHE | 388 | 21.188 | 13.470 | 23.141 | 1.00 | 29.70 | BLGL |
| ATOM | 2936 | O | PHE | 388 | 20.176 | 13.496 | 22.424 | 1.00 | 29.14 | BLGL |
| ATOM | 2937 | N | GLN | 389 | 22.125 | 14.412 | 23.102 | 1.00 | 31.10 | BLGL |
| ATOM | 2938 | CA | GLN | 389 | 22.022 | 15.532 | 22.174 | 1.00 | 32.46 | BLGL |
| ATOM | 2939 | CB | GLN | 389 | 22.603 | 16.797 | 22.793 | 1.00 | 35.41 | BLGL |
| ATOM | 2940 | CG | GLN | 389 | 22.086 | 17.088 | 24.177 | 1.00 | 44.69 | BLGL |
| ATOM | 2941 | CD | GLN | 389 | 22.807 | 18.261 | 24.818 | 1.00 | 50.70 | BLGL |
| ATOM | 2942 | OE1 | GLN | 389 | 22.674 | 19.401 | 24.372 | 1.00 | 52.70 | BLGL |
| ATOM | 2943 | NE2 | GLN | 389 | 23.588 | 17.985 | 25.866 | 1.00 | 53.54 | BLGL |
| ATOM | 2944 | C | GLN | 389 | 22.779 | 15.221 | 20.893 | 1.00 | 30.30 | BLGL |
| ATOM | 2945 | O | GLN | 389 | 22.270 | 15.416 | 19.790 | 1.00 | 31.42 | BLGL |
| ATOM | 2946 | N | TYR | 390 | 23.993 | 14.715 | 21.051 | 1.00 | 28.80 | BLGL |
| ATOM | 2947 | CA | TYR | 390 | 24.851 | 14.403 | 19.917 | 1.00 | 30.88 | BLGL |
| ATOM | 2948 | CB | TYR | 390 | 26.204 | 13.911 | 20.427 | 1.00 | 35.50 | BLGL |
| ATOM | 2949 | CG | TYR | 390 | 26.963 | 14.956 | 21.217 | 1.00 | 41.72 | BLGL |
| ATOM | 2950 | CD1 | TYR | 390 | 28.151 | 14.632 | 21.871 | 1.00 | 45.09 | BLGL |
| ATOM | 2951 | CE1 | TYR | 390 | 28.861 | 15.595 | 22.603 | 1.00 | 47.24 | BLGL |
| ATOM | 2952 | CD2 | TYR | 390 | 26.496 | 16.273 | 21.313 | 1.00 | 42.36 | BLGL |
| ATOM | 2953 | CE2 | TYR | 390 | 27.192 | 17.240 | 22.043 | 1.00 | 45.40 | BLGL |
| ATOM | 2954 | CZ | TYR | 390 | 28.376 | 16.894 | 22.686 | 1.00 | 47.41 | BLGL |
| ATOM | 2955 | OH | TYR | 390 | 29.078 | 17.841 | 23.406 | 1.00 | 46.59 | BLGL |
| ATOM | 2956 | C | TYR | 390 | 24.298 | 13.425 | 18.889 | 1.00 | 29.06 | BLGL |
| ATOM | 2957 | O | TYR | 390 | 24.591 | 13.553 | 17.704 | 1.00 | 29.24 | BLGL |
| ATOM | 2958 | N | VAL | 391 | 23.508 | 12.450 | 19.324 | 1.00 | 27.33 | BLGL |
| ATOM | 2959 | CA | VAL | 391 | 22.943 | 11.488 | 18.381 | 1.00 | 25.21 | BLGL |
| ATOM | 2960 | CB | VAL | 391 | 22.008 | 10.476 | 19.087 | 1.00 | 23.42 | BLGL |
| ATOM | 2961 | CG1 | VAL | 391 | 22.803 | 9.635 | 20.061 | 1.00 | 19.38 | BLGL |
| ATOM | 2962 | CG2 | VAL | 391 | 20.886 | 11.202 | 19.805 | 1.00 | 21.53 | BLGL |
| ATOM | 2963 | C | VAL | 391 | 22.154 | 12.226 | 17.299 | 1.00 | 26.03 | BLGL |
| ATOM | 2964 | O | VAL | 391 | 22.028 | 11.749 | 16.175 | 1.00 | 23.37 | BLGL |
| ATOM | 2965 | N | ASP | 392 | 21.635 | 13.400 | 17.647 | 1.00 | 27.71 | BLGL |
| ATOM | 2966 | CA | ASP | 392 | 20.862 | 14.200 | 16.710 | 1.00 | 30.77 | BLGL |
| ATOM | 2967 | CB | ASP | 392 | 20.134 | 15.323 | 17.448 | 1.00 | 32.83 | BLGL |
| ATOM | 2968 | CG | ASP | 392 | 18.986 | 14.820 | 18.302 | 1.00 | 34.68 | BLGL |
| ATOM | 2969 | OD1 | ASP | 392 | 18.444 | 15.617 | 19.103 | 1.00 | 35.32 | BLGL |

# Fig. 4 cont.

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ATOM    2970  OD2 ASP   392      18.618  13.636  18.167  1.00 35.22          BLGL
ATOM    2971  C   ASP   392      21.731  14.818  15.621  1.00 33.35          BLGL
ATOM    2972  O   ASP   392      21.467  14.650  14.430  1.00 35.61          BLGL
ATOM    2973  N   THR   393      22.777  15.526  16.035  1.00 34.96          BLGL
ATOM    2974  CA  THR   393      23.664  16.215  15.105  1.00 34.87          BLGL
ATOM    2975  CB  THR   393      23.998  17.626  15.602  1.00 35.87          BLGL
ATOM    2976  OG1 THR   393      24.820  17.526  16.774  1.00 37.14          BLGL
ATOM    2977  CG2 THR   393      22.726  18.392  15.952  1.00 35.93          BLGL
ATOM    2978  C   THR   393      24.991  15.518  14.908  1.00 36.53          BLGL
ATOM    2979  O   THR   393      25.462  15.358  13.787  1.00 36.72          BLGL
ATOM    2980  N   GLY   394      25.596  15.115  16.014  1.00 38.00          BLGL
ATOM    2981  CA  GLY   394      26.896  14.481  15.961  1.00 38.77          BLGL
ATOM    2982  C   GLY   394      27.828  15.442  16.679  1.00 40.97          BLGL
ATOM    2983  O   GLY   394      27.389  16.494  17.143  1.00 40.87          BLGL
ATOM    2984  N   THR   395      29.105  15.107  16.787  1.00 43.10          BLGL
ATOM    2985  CA  THR   395      30.043  15.990  17.461  1.00 45.02          BLGL
ATOM    2986  CB  THR   395      30.967  15.197  18.393  1.00 43.84          BLGL
ATOM    2987  OG1 THR   395      31.206  13.896  17.840  1.00 43.18          BLGL
ATOM    2988  CG2 THR   395      30.340  15.054  19.753  1.00 41.53          BLGL
ATOM    2989  C   THR   395      30.883  16.752  16.443  1.00 48.88          BLGL
ATOM    2990  O   THR   395      31.470  16.155  15.536  1.00 49.70          BLGL
ATOM    2991  N   PRO   396      30.941  18.089  16.578  1.00 52.29          BLGL
ATOM    2992  CD  PRO   396      30.225  18.889  17.594  1.00 52.46          BLGL
ATOM    2993  CA  PRO   396      31.712  18.955  15.672  1.00 52.98          BLGL
ATOM    2994  CB  PRO   396      31.537  20.343  16.291  1.00 53.36          BLGL
ATOM    2995  CG  PRO   396      30.173  20.256  16.948  1.00 52.73          BLGL
ATOM    2996  C   PRO   396      33.188  18.543  15.578  1.00 53.94          BLGL
ATOM    2997  O   PRO   396      33.678  18.369  14.436  1.00 54.55          BLGL
END
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                   9          19         29         39
---------- ---------- -ALTYRGVDW SSVVVEERAG VSYKNTNGNA QPLENILAAN   39 MT
---------- ---------- -ALQYKGVDW SSVMVEERAG VRYKNVNGQE KPLEYILAEN   39 HI
---------- ---------- -ALTYRGADI SSLLLLEDEG YSYKNLNGQT QALETILADA   39 AA
AHRDSGTAKS GLYVEKVSGL RKDFIKGVDV SSIIALEESG VAFYNESGKK QDIFNTLKEA   60 BL
   10         20         30         40         50         60


   49         54         61         71         81         91
GVNTVRQRVW VNPAD----- ---GNYNLDY NIAIAKRAKA AGLGVYIDFH YSDTWADPAH   91
GVNMVRQRVW VNPWD----- ---GNYNLDY NIQLARRAKA AGLGLYINFH YSDTWADPAH   91
GINSIRQRVW VNPSD----- ---GSYDLDY NLELAKRVKA AGMSLYLDLH LSDTWADPSD   91
GVNYVRVRIW NDPYDANGNG YGGGNNDLEK AIQIGKRANA NGMKLLADFH YSDFWADPAK  120
   70         80         90        100        110        120


  100        110        120        130        140        150
QTMPAGWP-S DIDNLSWKLY NYTLDAANKL QNAGIQPTIV SIGNEIRAGL LWPTGRTENW  150
QTTPAGWP-S DINNLAWKLY NYTLDSMNRF ADAGIQVDIV SIGNEITQGL LWPLGKTNNW  150
QTTPSGWSTT DLGTLKWQLY NYTLEVCNTF AENDIDIEII SIGNEIRAGL LWPLGETSSY  151
QKAPKAWANL NFEDKKTALY QYTKQSLKAM KAAGIDIGMV QVGNETNGGL A----GETDW  176
  130        140        150        160        170        176


  160        170        180        190        200        210
ANIARLLHSA AWGIKDSSLS PKPKIMIHLD NGWDWGTQNW WYTNVLKQGT LELSDFDMMG  210
YNIARLLHSA AWGVKDSRLN PKPKIMVHLD NGWNWDTQNW WYTNVLSQGP FEMSDFDMMG  210
SNIGALLHSG AWGVKDSNLA TTPKIMIHLD DGWSWDQQNY FYETVLATGE LLSTDFDYFG  211
AKMSQLFNAG SQAVRETD-- SNILVALHFT NPETSGRYAW IAETLHRH-- --HVDYDVFA  230
  186                   204        214                   230


  220        230        240        250        255        265
VSFYPFYSSS ATLSALKSSL DNMAKTWNKE IAVVETNWPI SC-----PNP RYSFPSDVKN  265
VSFYPFYSAS ATLDSLRRSL NNMVSRWGKE VAVVETNWPT SC-----PYP RYQFPADVRN  265
VSYYPFYSAS ATLASLKTSL ANLQSTYDKP VVVVETNWPV SC-----PNP AYAFPSDLSS  266
SSYYPFW--H GTLKNLTSVL TSVADTYGKK VMVAETSYTY TAEDGDHGN TAPKNGQTLN  288
  238        248        258        268        278        288


  275        285        294
IPFSPEGQTT FITNVANIVS SVS-RGVGLF YWEPAWIH-- ---------- ----------  302
VPFSAAGQTQ YIQSVANVVS SVS-KGVGLF YWEPAWIH-- ---------- ----------  302
IPFSVAGQQE FLEKLAAVVE ATT-DGLGVY YWEPAWIG-- ---------- ----------  303
NPVTVQGQAN AVRDVIQAVS DVGEAGIGVF YWEPAWIPVG PAHRLEKNKA LWETYGSGWA  348
  298        308        318        328        338        348


             309        318        328
---------- ---NANLGSS CADNTMFSQ- SGQALSSLSV FQRI------ --          332
---------- ---NANLGSS CADNTMFTP- SGQALSSLSV FHRI------ --          332
---------- ---NAGLGSS CADNLMVDYT TDEVYESIET LGEL------ --          334
TSYAAEYDPE DAGKWFGGSA VDNQALFDF- KGRPLPSLHV FQYVDTGTPF KN          399
  358        368        377        387        397
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**Fig. 5**

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                   9         19        29        39
---------- ---------- -ALTYRGVDW SSVVVEERAG VSYKNTNGNA QPLENILAAN 39 MT
---------- ---------- -ALQYKGVDW SSVMVEERAG VRYKNVNGQE KPLEYILAEN 39 HI
---------- ---------- -ALTYRGADI SSLLLLEDEG YSYKNLNGQT QALETILADA 39 AA
AHRDSGTAKS GLYVEKVSGL RKDFIKGVDV SSIIALEESG VAFYNESGKK QDIFNTLKEA 60 BL
---------- ---------- -ALTYRGADI SSLLIEEDAG ISYKNLNGET QALEDILVNN 39 AT
---------- --------M NKDFIKGADV SSVIALENSG VTFYNTNGKR QDIFTTLKQA 41 BS
---------- ----NTGVAD NTPFYVGADL SYVNEMESCG ATYRD-QGKK VDPFQLFADK 45 PF
            6         16        26        35        45


          49        54              61        71        81        91
GVNTVRQRVW VNPAD----- ---GNYNLDY NIAIAKRAKA AGLGVYIDFH YSDTWADPAH 91
GVNMVRQRVW VNPWD----- ---GNYNLDY NIQLARRAKA AGLGLYINFH YSDTWADPAH 91
GINSIRQRVW VNPSD----- ---GSYDLDY NLELAKRVKA AGMSLYLDLH LSDTWADPSD 91
GVNYVRVRIW NDPYDANGNG YGGGNNDLEK AIQIGKRANA NGMKLLADFH YSDFWADPAK 120
GVNSIRQRVW VDPSD----- ---GSYDLDY NLKLAKRVQA AGMSIYLDLH LSDTWADPSD 91
GVNYVRVRIW NHPYDSNGNG YGGGNNDVQK AIEIGKRATA NGMKVLADFH YSDFWADPAK 101
GADLVRVRLW HNATWT---- ---KYSDLKD VSKTLKRAKN AGMKTLLDFH YSDTWTDPEK 98
            55        61        68        78        88        98


          99        109       119       129       139       145
QTMPAGWP-- SDIDNLSWKL YNYTLDAANK LQNAGIQPTI VSIGNEIRAG LLWPTG---- 145
QTTPAGWP-- SDINNLAWKL YNYTLDSMNR FADAGIQVDI VSIGNEITQG LLWPLG---- 145
QTTPSGWST- TDLGTLKWQL YNYTLEVCNT FAENDIDIEI ISIGNEIRAG LLWPLG---- 146
QKAPKAWAN- LNFEDKKTAL YQYTKQSLKA MKAAGIDIGM VQVGNETNGG LA-------- 171
QTTPTGWST- TDIDTLTWQL YNYTLEVCNT FAENDIDVEI VSIGNEISSG LLWPLG---- 146
QKVPKAWAN- LSFEAKKAKL YEYTKQSLQK MIKEGVDIGM VQVGNETTGG FA-------- 152
QFIPKAWAHI TDTKELAKAL YDYTTDTLAS LDQQQLLPNL VQVGNETNIE ILQAEDTLVH 158
           109       118       128       138       148       158


          155       165       175       185       195       205
RTENWANIAR LLHSAAWGIK DSSLSPKPKI MIHLDNGWDW GTQNWWYTNV LKQGTLELSD 205.
KTNNWYNIAR LLHSAAWGVK DSRLNPKPKI MVHLDNGWNW DTQNWWYTNV LSQGPFEMSD 205
ETSSYSNIGA LLHSGAWGVK DSNLATTPKI MIHLDDGWSW DQQNYFYETV LATGELLSTD 206
GETDWAKMSQ LFNAGSQAVR ETD--SNILV ALHFTNPETS GRYAWIAETL HRH----HVD 225
KTSNYDNIAK LLHSGAWGVK DSDLTTTPKI MIHLDNGWDW DEQEYFYKTV LATGSLLSTD 206
GETDWTKMCQ LFNEGSRAVR ETN--SNILV ALHFTNPETA GRYSFIAETL SKN----KVD 206
GIPNWQRNAT LLNSGVNAVR DYSKKTGKPI QVVLHIAQPE NALWWFKQAK ENG----VID 214
           168       178       188       198       208       214


          215       225       235       245       252       260
FDMMGVSFYP FYSSSATLSA LKSSLDNMAK TWNKEIAVVE TNWPISC--- --PNPRYSFP 260
FDMMGVSFYP FYSASATLDS LRRSLNNMVS RWGKEVAVVE TNWPTSC--- --PYPRYQFP 260
FDYFGVSYYP FYSASATLAS LKTSLANLQS TYDKPVVVVE TNWPVSC--- --PNPAYAFP 261
YDVFASSYYP FW--HGTLKN LTSVLTSVAD TYGKKVMVAE TSYTYTAEDG DGHGNTAPKN 283
FDLMGVSYYP FYSSEATLSS LKTSLTNMQS NYDKPVVVVE TNWPVSC--- --PDPEYSFP 261
YDVFASSYYP FW--HGTLQN LTSVLKAVAN TYGKKVMVAE TSYTYTAEDG DGHGNTAPKS 264
YDVIGLSYYP QWS-EYSLPQ LPDAIAELQN TYHKPVMIVE TAYPWTLHNF DQAGNVLGEK 273
           224       233       243       253       263       273


          270       280       289       299
SDVKNIPFSP EGQTTFITNV ANIVSSVS-R GVGLFYWEPA WIH------- ---------- 302
ADVRNVPFSA AGQTQYIQSV ANVVSSVS-K GVGLFYWEPA WIH------- ---------- 302
SDLSSIPFSV AGQQEFLEKL AAVVEATT-D GLGVYYWEPA WIG------- ---------- 303
GQTLNNPVTV QGQANAVRDV IQAVSDVGEA GIGVFYWEPA WIPVGPAHRL EKNKALWETY 333
SDLTSIPFSA AGQEEFLEKL AEVVEGVT-D GLGIYYWEPA WID------- ---------- 303
GQTLPYPISV QGQATAVRDV MEAVANTGKA GLGVFYWEPA WIPVGPKTQI EKNKVLWETY 314
AVQPEFPASP RGQLTYLLTL TQLVKSAG-- GMGVIYWEPA WVSTRCR--- ---------- 318
           283       293       301       311
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# Fig. 6

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```
                       314          322          332
---------- --------NA NLGSSCADNT MFSQ--SGQA LSSLSVFQRI --------   332
---------- --------NA NLGSSCADNT MFTP--SGQA LSSLSVFHRI --------   332
---------- --------NA GLGSSCADNL MVDYT-TDEV YESIETLGEL --------   334
GSGWATSYAA EYDPEDAGKW FGGSAVDNQA LFDF--KGRP LPSLHVFQYV DTGTPFKN   399
---------- --------NA GLGSSCADNL MVDVN-TDEV LESVTVFEDL --------   334
GSGWASSYAA EYDPEDAGKW YGGSAVDNQA LFDF--NGHP LPSLQVFQYA --------   372
---------- -------TLW GKGSHWENAS FFDATRKNNA LPAFLFFKAD YQASAQAE   359
                       321          331          341          351
```

# Fig. 6 cont.